

ON THE STABILITY OF CRYSTAL LATTICES.

Being

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by

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ON THE STABILITY OF CRYSTAL LATTICES.

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ON THE STABILITY OF CRYSTAL LATTICES.

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ON THE STABILITY OF CRYSTAL LATTICES.

Introduction.

The usual method of investigating the stability of a crystal lattice consists in comparing its energy with that of other possible lattices built from the same particles. The results obtained are rather meagre (Born and Goepper-Mayer (5) -) since the calculations are rather tedious and hardly reliable owing to the fact that the differences of the lattice energies are small. On the other hand Goldschmidt (9) has very successfully predicted the lattice type of ionic and other lattices from no other knowledge than that of the radii of the atoms or ions concerned. Generalizing the idea of densest packing which holds for equal particles he assumes that the most stable configuration of two different kinds of particles is that lattice in which each particle has a maximum number of neighbours (coordination number) of the other kind in the shortest distance possible. Though this geometrical principle is very plausible there is no satisfactory dynamical justification.

In common dynamical problems of stability we have apart from the method of comparing the absolute values of energy the well known method of small vibrations. The application of this method to the case of crystals seems to be difficult since the number of normal vibrations is practically

infinite. The complete vibrational spectrum must be worked out and this has only been tried for a few special cases. { Blackmann (2), Herzfeld and Lyddane (11), Kellermann (14) }.

It is well known that monatomic lattices are generally face centred cubic (f); there occur a few body centred ones (b), while the simple cubic lattices (s) seem not to exist.* How can this be explained? Goldschmidt's principle mentioned in the beginning gives the answer; the face centred cubic lattice is a densest packing of equal spheres.

We can go a little further by introducing the coordination number (number of its first neighbours); its value for the three lattice types is (f) = 12, (b) = 8, (s) = 6. This order corresponds just to the degree of stability which is explained by the consideration that the first neighbours give the greatest contribution to the lattice energy so that the energy is approximately proportional to their number. But this argument

* There exist other types of monatomic lattices as diamond and graphite which are in some cases of a very high stability. These cases cannot be treated as particles with central forces.

is exposed to the objection that this preponderating importance of the first neighbours is not proved, and is not always the case, as the existence of body centred lattices shows.

Born (3) has shown that the stability criterion based on the quadratic terms of the deformation energy gives an answer which depends also on the coordination number, but it is of a more qualitative character. He has derived the stability criteria for the three cubic lattices of the Bravais type under the assumption of central forces of a very general type. The result obtained is that the face centred lattice which corresponds to densest packing is completely stable; the body centred lattice only under certain conditions (small exponent of the law of force) whereas the simple lattice is always unstable.

Prof. Born suggested to me to verify these results by complete calculation of the elastic constants for a special law of force, namely that where the potential energy consists of two terms one attractive and proportional to r^{-m} and the other repulsive and proportional to r^{-n} , $n > m$. In my paper "On the stability of Crystal lattices, part II" (15) (in the press) I have taken the conditions of stability developed in part I by Born (3) (also in the press) and expressed them in the form that two functions of the number n are monotone increasing. I have numerically

worked out these functions and represented them as curves of the argument n . The result thus obtained by a method different from that of Born is in complete agreement with what he obtained in part I.

Besides investigating the stability criteria I had two other objects in view, viz. to improve, if possible, the existing laborious methods of calculating the lattice sum $S_n^{(a)}$ and secondly to find out a suitable method for calculating another type of lattice sum $S_n^{(a)}$ which had not been calculated so far, but would be found very useful in work on crystal lattices. Both the objects have been achieved.

In the course of my calculations I have come across the integral $\int_1^\infty \beta^m e^{-\beta x} d\beta$ which I have denoted by $\phi_m(x)$. Here $m = \pm \frac{p}{2}$ where $p = 0, 1, 2, 3, \dots$ and $x = \frac{b\pi}{4}$, where m and x being independent of each other. As these ϕ_m 's are likely to be useful I have tabulated their values for various m 's and x 's.

In this dissertation I have included for clarity and continuity certain portions of Born's paper (3) the manuscript copy of which he very kindly lent to me for my use. I take this opportunity of expressing my sincere thanks to Prof. Born for sharing with me his ideas and calculations and interest in my work.

CHAPTER I.

The elasticity constants.

Let a be the absolute value of the component of the vector distance of neighbours in the direction of the cubic axes. Then the lattice points of the undistorted cubic lattice are given by the vectors

$$(1.1) \quad \underline{r}^{ol} = l_1 a, l_2 a, l_3 a$$

The cube with side a may be deformed into the parallelepiped with sides $\underline{a}_1, \underline{a}_2, \underline{a}_3$; then the lattice points of the deformed lattice are given by

$$(1.2) \quad \underline{r}^l = l_1 \underline{a}_1 + l_2 \underline{a}_2 + l_3 \underline{a}_3$$

The integers l_1, l_2, l_3 assume different sets of values for the three Bravais types (s), (f), (b), viz., (s): all possible positive and negative integral values of l_1, l_2 and l_3 ; (f): all the three even, or one even and two odd; (b): all the three even or all the three odd.

We introduce certain notations

which are all explained at their proper places. Thus we write for the square of the distance from the origin

$$(1.3) \quad (\underline{r}^l)^2 = (l_1 \underline{a}_1 + l_2 \underline{a}_2 + l_3 \underline{a}_3)^2 = \sum_{\alpha\beta} \underline{a}_{\alpha\beta} l_{\alpha} l_{\beta}$$

with

$$(1.4) \quad \underline{a}_{\alpha\beta} = \underline{a}_{-\alpha} \cdot \underline{a}_{\beta}$$

and also

$$(1.5) \quad (\underline{r}^l)^2 = (\underline{r}^{ol})^2 + 2\rho^l$$

Where $2\rho^L$ is the increase in the value of $(\underline{r}^{oL})^2$ due to deformation of the lattice, and therefore

$$(1.6) \quad 2\rho^L = l_1^2 (\underline{a}_1^2 - a^2) + l_2^2 (\underline{a}_2^2 - a^2) + l_3^2 (\underline{a}_3^2 - a^2) + 2l_2 l_3 (\underline{a}_2 \cdot \underline{a}_3) \\ + 2l_3 l_1 (\underline{a}_3 \cdot \underline{a}_1) + 2l_1 l_2 (\underline{a}_1 \cdot \underline{a}_2)$$

This we write as

$$(1.7) \quad 2\rho^L = \sum_{\alpha\beta} \delta a_{\alpha\beta} l_\alpha l_\beta$$

The $\delta a_{\alpha\beta}$ are connected with the strain components $e_{\alpha\beta}$ of the usual elastic theory by

$$(1.8) \quad \delta a_{\alpha\beta} = a^2 e_{\alpha\beta}$$

or using Voigt's symbol $2x_x = e_{11}, \dots, y_z = e_{23}, \dots$

$$(1.9) \quad \begin{cases} 2x_x = e_{11} = \frac{\delta a_{11}}{a^2} = \frac{a_1^2 - a^2}{a^2} ; \dots \\ y_z = e_{23} = \frac{\delta a_{23}}{a^2} = \frac{a_2 \cdot a_3}{a^2} , \dots \end{cases}$$

We definitely assume the forces between the atoms to be central having the potential energy $\phi(r)$.

Now

$$(1.10) \quad \frac{d}{d\rho} \phi(\sqrt{r^2 + 2\rho}) = \frac{d\phi(\sqrt{r^2 + 2\rho})}{d(\sqrt{r^2 + 2\rho})} \cdot \frac{1}{\sqrt{r^2 + 2\rho}}$$

Introducing the operator

$$(1.11) \quad D = \frac{1}{r} \frac{d}{dr}$$

We write (1.10) as

$$(1.12) \quad \frac{d}{d\rho} \phi(\sqrt{r^2 + 2\rho}) = (D\phi)_{r=\sqrt{r^2 + 2\rho}}$$

We now expand $\phi(\sqrt{r^2 + 2\rho})$ in a series of

ascending powers of ρ , we get

$$(1.13) \quad \phi(\sqrt{r^2 + 2\rho}) = \phi + \rho D\phi + \frac{1}{2}\rho^2 D^2\phi + \dots$$

the argument of ϕ being r

The total potential energy of the lattice, neglecting surface effects, is

$$(1.14) \quad U = \frac{1}{2} N \sum_l \phi(r^l)$$

Substituting the value of r^l from (1.5) and applying (1.13) we get

$$(1.15) \quad U = \frac{1}{2} N \sum_l \left\{ \phi^l + \rho D\phi^l + \frac{1}{2}\rho^2 D^2\phi^l + \dots \right\}$$

where $\phi^l, D\phi^l$ etc. represent the values of the functions $\phi(r), D\phi(r), \dots$ for $r = r^{\circ l}$.

We now substitute the value of ρ^l from (1.7) and get

$$(1.16) \quad U = \frac{1}{2} N \sum_l \phi^l + \frac{1}{4} N \sum_{\alpha\beta} \delta_{\alpha\beta} \sum_l l_\alpha l_\beta D\phi^l \\ + \frac{1}{16} N \sum_{\alpha\beta\mu\nu} \delta_{\alpha\beta} \delta_{\mu\nu} \sum_l l_\alpha l_\beta l_\mu l_\nu D^2\phi^l + \dots$$

Owing to the cubic symmetry all lattice sums containing odd powers of l_1, l_2, l_3 are zero, and those lattice sums which can be transformed into one another by exchanging the indices of l_1, l_2 and l_3 are equal. Therefore, only the following lattice sums (over the undeformed lattice) occur:

$$(1.17) \quad \left(\begin{matrix} k \\ \mu\nu \end{matrix} \right) = \sum_l D^k \phi^l l_1^{2\mu} l_2^{2\nu},$$

and we can easily put

$$(1.18) \quad U = U_0 + U_1 + U_2 + \dots$$

where

$$\begin{aligned}
 U_0 &= \frac{1}{2} N \begin{pmatrix} 0 \\ 0 \end{pmatrix} \\
 U_1 &= \frac{1}{4} N \begin{pmatrix} 1 \\ 0 \end{pmatrix} \sum_{\alpha} \delta a_{\alpha\alpha} \\
 U_2 &= \frac{1}{16} N \left\{ \begin{pmatrix} 2 \\ 2 \end{pmatrix} \sum_{\alpha} (\delta a_{\alpha\alpha})^2 + \begin{pmatrix} 2 \\ 1 \end{pmatrix} \sum_{\alpha\beta} (\delta a_{\alpha\alpha} \delta a_{\beta\beta} + 2 (\delta a_{\alpha\beta})^2) \right\}.
 \end{aligned}
 \tag{1.19}$$

The usual stability criterion consists in comparing the values of

$$U_0 = \frac{1}{2} N \sum_l \epsilon^l
 \tag{1.20}$$

for different lattices. Instead, we consider the quadratic form U_2 in which the following combinations of strain components occur

$$\begin{aligned}
 \sum_{\alpha} (\delta a_{\alpha\alpha})^2 &= \delta a_{11}^2 + \delta a_{22}^2 + \delta a_{33}^2 = a^4 (e_{11}^2 + e_{22}^2 + e_{33}^2) = 4a^4 (x_x^2 + y_y^2 + z_z^2) \\
 \sum_{\alpha\beta} \delta a_{\alpha\alpha} \delta a_{\beta\beta} &= 2 (\delta a_{22} \delta a_{33} + \dots) = 2a^4 (e_{22} e_{33} + \dots) = 8a^4 (y_y z_z + \dots) \\
 \sum_{\alpha\beta} (\delta a_{\alpha\beta})^2 &= 2 (\delta a_{23}^2 + \dots) = 2a^4 (e_{23}^2 + \dots) = 2a^4 (y_y^2 + z_z^2 + x_x^2).
 \end{aligned}
 \tag{1.21}$$

The density of elastic energy of a cubic crystal in Voigt's (18) notation is

$$\begin{aligned}
 u = \frac{U_2}{v N} &= \frac{1}{2} c_{11} (x_x^2 + y_y^2 + z_z^2) \\
 &\quad + c_{12} (y_y z_z + z_z x_x + x_x y_y) \\
 &\quad + \frac{1}{2} c_{44} (y_y^2 + z_z^2 + x_x^2),
 \end{aligned}
 \tag{1.22}$$

where v is the volume containing one particle.

If we write $v = \gamma a^3$, γ varies for the different lattice types $\{(s): \gamma = 1, (b): \gamma = 4, (f): \gamma = 2\}$.

By comparing (1.19) with (1.22) we get for the elasticity constants the expressions

$$(1.23) \quad \begin{aligned} c_{11} &= \frac{1}{2} \frac{a}{\gamma} \binom{2}{20} = \frac{1}{2} \frac{a}{\gamma} \sum_l D^2 \phi^l l_1^4 \\ c_{12} = c_{44} &= \frac{1}{2} \frac{a}{\gamma} \binom{2}{11} = \frac{1}{2} \frac{a}{\gamma} \sum_l D^2 \phi^l l_1^2 l_2^2 \end{aligned}$$

The equality of c_{12} and c_{44} is in agreement with the well known fact, that central forces in a monatomic lattice lead to Cauchy's relations.

We assume the potential energy between the particles to be

$$(1.24) \quad \phi = u \frac{nm}{n-m} \left(-\frac{1}{m} \frac{r_0^m}{r^m} + \frac{1}{n} \frac{r_0^n}{r^n} \right);$$

then

$$(1.25) \quad D\phi = u \frac{nm}{n-m} \frac{1}{r_0^2} \left(-\frac{(n+2)r_0^{n+2}}{r^{n+2}} + \frac{(m+2)r_0^{m+2}}{r^{m+2}} \right),$$

and

$$(1.26) \quad D^2 \phi = u \frac{nm}{n-m} \frac{1}{r_0^4} \left(-\frac{(n+2)r_0^{n+4}}{r^{n+4}} + \frac{(m+2)r_0^{m+4}}{r^{m+4}} \right).$$

Here r_0 is the equilibrium distance of the two particles since $D\phi = 0$ for $r = r_0$. $u = -\phi$ is the dissociation energy.

We introduce the lattice sums

(1.27)

$$S_p^{(0)} = \sum_l' \frac{1}{(l_1^2 + l_2^2 + l_3^2)^{p/2}} \quad ; \quad S_p^{(1)} = \sum_l' \frac{l_3^2}{(l_1^2 + l_2^2 + l_3^2)^{p/2}}$$

$$S_p^{(2)} = \sum_l' \frac{l_3^4}{(l_1^2 + l_2^2 + l_3^2)^{p/2}} \quad ; \quad S_p^{(3)} = \sum_l' \frac{l_2^2 l_3^2}{(l_1^2 + l_2^2 + l_3^2)^{p/2}}$$

Between these quantities one has obviously the identities

$$(1.28) \quad 3 \int_p^{(1)} = \int_{p-2}^{(0)}$$

$$3 \int_p^{(2)} + 6 \int_p^{(3)} = \int_{p-4}^{(0)}$$

The equilibrium condition $D\phi=0$ then becomes

$$(1.29) \quad \left(\frac{a}{r_0}\right)^{n-m} = \frac{\int_{n+2}^{(1)}}{\int_{m+2}^{(1)}} \quad ?$$

and the elasticity constants expressed in terms of these S's are

$$(1.30) \quad C_{11} = \frac{a^4}{2\nu} \binom{2}{20} = \frac{u}{2\nu} \frac{nm}{n-m} \left(-(m+2) \left(\frac{r_0}{a}\right)^m \int_{m+4}^{(2)} + (n+2) \left(\frac{r_0}{a}\right)^n \int_{n+4}^{(2)} \right)$$

$$C_{44} = C_{12} = \frac{a^4}{2\nu} \binom{2}{11}$$

$$= \frac{u}{2\nu} \frac{nm}{n-m} \left(-(m+2) \left(\frac{r_0}{a}\right)^m \int_{m+4}^{(3)} + (n+2) \left(\frac{r_0}{a}\right)^n \int_{n+4}^{(3)} \right)$$

Here we can eliminate $\frac{a}{r_0}$ with the help

of (1.29); then the elasticity constants divided by the common factor $\frac{\mu}{2\nu}$ are functions of n and m alone.

CHAPTER II.

Stability of the three cubic lattices.

Stability conditions are derived from the positiveness of the expression (1.22). Its characteristic determinant splits up into products

$$(2.1) \quad \begin{vmatrix} c_{11} - \lambda & c_{12} & c_{12} \\ c_{12} & c_{11} - \lambda & c_{12} \\ c_{12} & c_{12} & c_{11} - \lambda \end{vmatrix} \begin{vmatrix} c_{44} - \lambda & 0 & 0 \\ 0 & c_{44} - \lambda & 0 \\ 0 & 0 & c_{44} - \lambda \end{vmatrix}$$

$$= (c_{11} + 2c_{12} - \lambda)(c_{11} - c_{12} - \lambda)^2 (c_{44} - \lambda)^3$$

Hence the stability conditions are

$$(2.2) \quad c_{11} + 2c_{12} > 0, \quad c_{11} - c_{12} > 0, \quad c_{44} > 0$$

Our problem is therefore to discuss the signs of these combinations of the lattice sums.

Using the expressions (1.30) one gets the following:-

$$c_{11} + 2c_{12} > 0 \quad \text{gives} \quad \frac{n+2}{m+2} \cdot \frac{\sum_{m+2}^{(1)}}{\sum_{n+2}^{(1)}} \cdot \frac{\sum_{n+4}^{(2)} + 2 \sum_{n+4}^{(3)}}{\sum_{m+4}^{(2)} + 2 \sum_{n+4}^{(3)}} > 1$$

$$c_{11} - c_{12} > 0 \text{ gives}$$

$$\frac{n+2}{m+2} \frac{\int_{n+2}^{(1)}}{\int_{n+2}^{(1)}} \frac{\int_{n+4}^{(2)} - \int_{n+4}^{(3)}}{\int_{n+4}^{(2)} - \int_{n+4}^{(3)}} > 1$$

(2.3)

$$c_{44} > 0 \text{ gives}$$

$$\frac{n+2}{m+2} \frac{\int_{n+2}^{(1)}}{\int_{n+2}^{(1)}} \frac{\int_{n+4}^{(3)}}{\int_{n+4}^{(3)}} > 1$$

The first inequality reduces on account of (1.28) to $n > m$ which is trivially fulfilled.

For expressing the other two inequalities we introduce the two functions

$$A(n) = (n+2) \frac{\int_{n+4}^{(2)} - \int_{n+4}^{(3)}}{\int_{n+2}^{(1)}}$$

(2.4)

$$B(n) = (n+2) \frac{\int_{n+4}^{(3)}}{\int_{n+2}^{(1)}}$$

Then the crystal is stable if

(2.5)

$$\left. \begin{array}{l} A(n) > A(m) \\ B(n) > B(m) \end{array} \right\} \text{ for } n > m$$

One can simplify the expression (2.4) with the help of (1.28). Let us substitute the values of $\int^{(1)}$ and $\int^{(3)}$ in terms of $\int^{(0)}$ and $\int^{(2)}$ into (2.4); we thus get

(2.6)

$$A(n) = \frac{n+2}{2} \left(9 \frac{S_{n+4}^{(2)}}{S_n^{(0)}} - 1 \right)$$

and

(2.7)

$$\beta(n) = \frac{n+2}{2} \left(1 - 3 \frac{S_{n+4}^{(2)}}{S_n^{(0)}} \right)$$

The stability problem is therefore reduced to the question whether these two functions are monotone increasing. It is to be remarked that the stability does not depend explicitly on the lattice constant.

CHAPTER III.

Calculation of the lattice sums.

Numerical calculations of the sum $S_p^{(0)}$ have been published by Jones and Ingham (13) with help of the use of Epstein Zeta functions. Although it seems possible to extend this method to the sums of the type $S_p^{(2)}$, I have preferred to use two other methods according to the magnitude of n . For large n the terms of the lattice sums are added up to a certain limit by direct summation method and the rest replaced by an integral as was done by Born and Bormann (4); but I have improved this method by calculating the upper and lower limits for the error committed. The second method is applicable for all $n \geq 4$ and has been used upto $n = 10$. It consists in using transformation formulae but in a different way as used by Ewald (8) and Moliere (16). This method is more efficient and convenient than any other I know of, for low values of n .

First summation method.

We write

$$(3.1) \quad S_n^{(0)} = \sum_{q=1}^{\infty} \frac{v_q^{(0)}}{q^{n/2}} = \sum_{q=1}^{p-1} \frac{v_q^{(0)}}{q^{n/2}} + R_n^{(0)}(p),$$

where $v_q^{(0)}$ is the number of neighbours at the distance $q^{1/2}$ and

$$(3.2) \quad R_n^{(0)}(p) = \sum_{q=p}^{\infty} \frac{v_q^{(0)}}{q^{n/2}}.$$

It will now be shown that

$$(3.3) \quad R_n^{(0)}(p) < \iiint_{x^2+y^2+z^2=p'} \frac{dx dy dz}{(x^2+y^2+z^2)^{n/2}} + 3 \iint_{x^2+y^2=p''} \frac{dx dy}{(x^2+y^2)^{n/2}} + 6 \int_{x=\sqrt{p'''}} \frac{dx}{x^n},$$

and

$$(3.4) \quad R_n^{(0)}(p) > \iiint_{x^2+y^2+z^2=p} \frac{dx dy dz}{(x^2+y^2+z^2)^{n/2}} - 3 \iint_{x^2+y^2=p} \frac{dx dy}{(x^2+y^2)^{n/2}} - 6 \int_{x=\sqrt{p}} \frac{dx}{x^n}.$$

Here the three terms correspond to those lattice points for which none or one or two coordinates are zero and the values of the lower limits p' , p'' and p''' (Table II) have to be determined with help of the Table I which gives the decomposition of any integer p into three squares $p = l_1^2 + l_2^2 + l_3^2$. Any decomposition of p is of one of the three types $l^2 + m^2 + n^2$ (space), $l^2 + m^2$ (plane), l^2 (axis); several of these may appear simultaneously. If one type or two do not appear we pick out the smallest of the numbers $p+1$, $p+2$, ... where the missing types appear, say p_1 and p_2 . Then in all these decompositions of p , and if necessary p_1 and p_2 , we reduce l , m and n by unity and add their squares. The smallest amongst those of the three types are p' , p'' and p''' .

Consider the space divided into unit cubic cells by lines drawn at unit distances parallel to the axes, x, y and z axes being respectively parallel to the directions of l_1 , l_2 and l_3 . Then corresponding to any one corner P_q of a cubic cell in space there will be one and only one value of

For the point P_q , $q = 3^2 + 2^2 = 13$; for $q = 5$ there are 8 points in the xy plane (24 points in space).

It is now obvious that in addition to the cubic cells we also require the unit squares on the coordinate planes and unit segments on coordinate axes so that every point corresponding to all possible values of q may have a cell or square or segment associated with it.

As P_q is the farthest corner of the cell (or square or segment) associated with it, we have for all points xyz in the cell (or square or segment)

$$(3.5) \quad \frac{1}{q^{1/2}} \leq \frac{1}{(x^2 + y^2 + z^2)^{1/2}}$$

The nearest corner will be $P_{q'}$ where $q' = (l-1)^2 + (m-1)^2 + (n-1)^2$.

We now replace the sum $\sum_{q=p}^{\infty} \frac{q^{(0)}}{q^{1/2}}$ by integrals over corresponding cells, squares and segments and get quite easily the inequality (3.3) viz.,

$$\sum_{q=p}^{\infty} \frac{q^{(0)}}{q^{1/2}} < \iiint_{x^2+y^2+z^2=p'} \frac{dx dy dz}{(x^2+y^2+z^2)^{1/2}} + 3 \iint_{x^2+y^2=p''} \frac{dx dy}{(x^2+y^2)^{1/2}} + 6 \int_{x^2=p'''} \frac{dx}{x}$$

To obtain the other inequality we this time associate with every corner that cell of which it is the nearest point. Every point on a coordinate plane can have two cells associated with it and every point on an axis, four cells. This means that on associating only one cell with every point we shall have some cells left unassociated, and

therefore, while integrating over the entire space, we must exclude the integrals over the unassociated cells. The entire first layer on one side of every coordinate plane will remain unassociated and so will a row of cells all along the length of every axis on the associated sides of the planes.

We can thus write

$$(3.6) \quad \sum_{q=p}^{\infty} \frac{v_q^{(0)}}{q^{n/2}} > \iiint_{x^2+y^2+z^2=p}^{\infty} \frac{dx dy dz}{(x^2+y^2+z^2)^{n/2}} - C$$

where C is the integral over the excluded space.

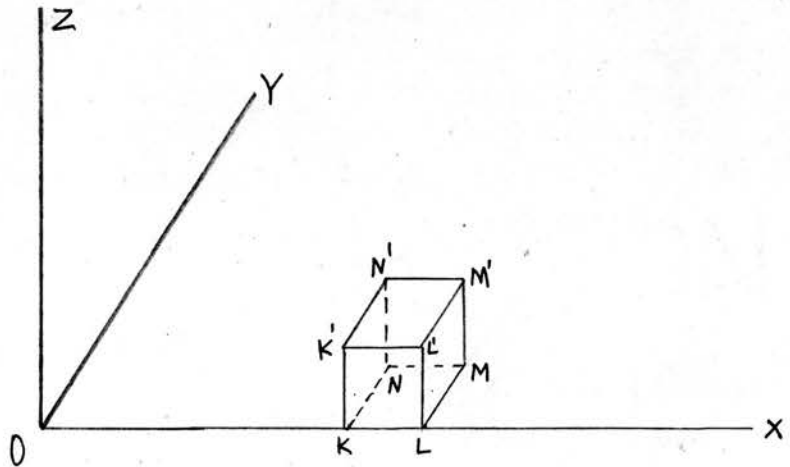


Fig. 2

Now from fig. 2 it is quite obvious that

$$(3.7) \quad \frac{1}{(OK)^n} > \int_{x=OK}^{OL} \frac{dx}{x^n} > \int_{x=OK}^{OL} \int_{y=0}^1 \frac{dy}{(x^2+y^2)^{n/2}} > \int_{x=OK}^{OL} \int_{y=0}^1 \int_{z=0}^1 \frac{dz}{(x^2+y^2+z^2)^{n/2}}$$

Using such inequalities to replace volume integrals over the excluded space i.e. first layers of cells over coordinate planes and rows of cells

along axes, by surface integrals over the planes and line integrals over axes, respectively, we get instead of (3.6) the inequality (3.4) viz.,

$$R_n^{(0)}(p) = \sum_{q=p}^{\infty} \frac{V_q^{(0)}}{q^{n/2}} > \iiint_{x^2+y^2+z^2=p} \frac{dx dy dz}{(x^2+y^2+z^2)^{n/2}} - 3 \iint_{x^2+y^2=p} \frac{dx dy}{(x^2+y^2)^{n/2}} - 6 \int_{x=\sqrt{p}}^{\infty} \frac{dx}{x^n}.$$

We denote these integrals by I and have

$$\begin{aligned} I_1(q) &= \iiint_{x^2+y^2+z^2=q} \frac{dx dy dz}{(x^2+y^2+z^2)^{n/2}} = \int_{\sqrt{q}}^{\infty} \frac{r^2 dr}{r^n} \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi = \frac{4\pi}{n-3} \frac{1}{q^{\frac{n-3}{2}}} \\ (3.8) \quad I_2(q) &= 3 \iint_{x^2+y^2=q} \frac{dx dy}{(x^2+y^2)^{n/2}} = 3 \int_{\sqrt{q}}^{\infty} \frac{r dr}{r^n} \int_0^{2\pi} d\phi = \frac{6\pi}{n-2} \frac{1}{q^{\frac{n-2}{2}}} \\ I_3(q) &= 6 \int_{\sqrt{q}}^{\infty} \frac{dx}{x^n} = \frac{6}{n-1} \frac{1}{q^{\frac{n-1}{2}}} \end{aligned}$$

Then we get from (3.3), (3.4) and (3.8)

$$\begin{aligned} (3.9) \quad I_1(p') - I_1(p) + I_2(p'') + I_3(p''') &> S_n^{(0)} - \left(\sum_{q=1}^{p-1} \frac{V_q^{(0)}}{q^{n/2}} + I_1(p) \right) \\ &> - (I_2(p) + I_3(p)) \end{aligned}$$

Similarly we write

$$(3.10) \quad S_n^{(2)} = \sum_{q=1}^{\infty} \frac{V_q^{(2)}}{q^{n/2}} = \sum_{q=1}^{p-1} \frac{V_q^{(2)}}{q^{n/2}} + R_n^{(2)}(p)$$

Here $V_q^{(2)}$ represents the sum of the fourth powers of l_3 of all points at distance $q^{\frac{1}{2}} = (l_1^2 + l_2^2 + l_3^2)^{\frac{1}{2}}$ from the origin; and

$$(3.11) \quad R_n^{(2)}(p) = \sum_{q=p}^{\infty} \frac{V_q^{(2)}}{q^{n/2}}$$

Then associating cells, squares and lengths with P_q as before, we get quite easily

$$(3.12) \quad \frac{l_3^4}{(l_1^2 + l_2^2 + l_3^2)^{n/2}} < \frac{(|r \cos \theta| + 1)^4}{r^n}$$

where r is any point in the cell, square or segment of which P_q ($q = l_1^2 + l_2^2 + l_3^2$) is the farthest point, and $|r \cos \theta|$ is the numerical value of $r \cos \theta$.

Also

$$(3.13) \quad \frac{l_3^4}{(l_1^2 + l_2^2 + l_3^2)^{n/2}} > \frac{(|r \cos \theta| - 1)^4}{r^n}$$

where r is any point in the cell, square or segment of which P_q is the nearest point.

On xy plane $l_3 = 0$ and consequently also on x and y axes.

Replacing sums by integrals we obtain

$$(3.14) \quad J_1^+(p') - J_1^-(p) + J_2^+(p'') + J_3^+(p''') > \sum_n^{(2)} - \left(\sum_{q=1}^{p-1} \frac{2}{q^{n/2}} + J_1^-(p) \right) \\ > - (J_2^-(p) + J_3^-(p))$$

where

$$J_1^+(p') = \int_{\sqrt{p'}}^{\infty} \int_0^{\pi} \frac{(|r \cos \theta| + 1)^4}{r^n} r^2 \sin \theta dr d\theta \int_0^{2\pi} d\phi$$

$$J_1^-(p) = \int_{\sqrt{p}}^{\infty} \int_0^{\pi} \frac{(|r \cos \theta| - 1)^4}{r^n} r^2 \sin \theta dr d\theta \int_0^{2\pi} d\phi$$

$$J_2^+(p'') = 2 \int_{\sqrt{p''}}^{\infty} \int_0^{\pi} \frac{(|r \cos \theta| + 1)^4}{r^n} r dr d\theta$$

$$J_2^-(p) = 2 \int_{\sqrt{p}}^{\infty} \int_0^{\pi} \frac{(|r \cos \theta| - 1)^4}{r^n} r dr d\theta$$

$$J_3^+(p''') = 2 \int_{\sqrt{p'''}}^{\infty} \frac{(z+1)^4}{z^n} dz$$

$$J_3^-(p) = 2 \int_{\sqrt{p}}^{\infty} \frac{(z-1)^4}{z^n} dz$$

On evaluating these integrals we get

$$J_1^+(p') = 4\pi \left[\frac{1}{5(n-7)(p')^{\frac{n-7}{2}}} + \frac{1}{(n-6)(p')^{\frac{n-6}{2}}} + \frac{2}{(n-5)(p')^{\frac{n-5}{2}}} \right. \\ \left. + \frac{2}{(n-4)(p')^{\frac{n-4}{2}}} + \frac{1}{(n-3)(p')^{\frac{n-3}{2}}} \right],$$

$$J_1^-(p) = 4\pi \left[\frac{1}{5(n-7)p^{\frac{n-7}{2}}} - \frac{1}{(n-6)p^{\frac{n-6}{2}}} + \frac{2}{(n-5)p^{\frac{n-5}{2}}} \right. \\ \left. - \frac{2}{(n-4)p^{\frac{n-4}{2}}} + \frac{1}{(n-3)p^{\frac{n-3}{2}}} \right],$$

$$J_2^+(p'') = \left[\frac{3\pi}{4(n-6)(p'')^{\frac{n-6}{2}}} + \frac{3\pi}{3(n-5)(p'')^{\frac{n-5}{2}}} + \frac{6\pi}{(n-4)(p'')^{\frac{n-4}{2}}} \right. \\ \left. + \frac{16}{(n-3)(p'')^{\frac{n-3}{2}}} + \frac{2\pi}{(n-2)(p'')^{\frac{n-2}{2}}} \right],$$

$$\bar{J}_2(p) = \left[\frac{3\pi}{4(n-6)p^{\frac{n-6}{2}}} - \frac{32}{3(n-5)p^{\frac{n-5}{2}}} + \frac{6\pi}{(n-4)p^{\frac{n-4}{2}}} - \frac{16}{(n-3)p^{\frac{n-3}{2}}} + \frac{2\pi}{(n-2)p^{\frac{n-2}{2}}} \right]$$

$$\frac{1}{3} J_3(p''') = 2 \left[\frac{1}{(n-5)(p''')^{\frac{n-5}{2}}} + \frac{4}{(n-4)(p''')^{\frac{n-4}{2}}} + \frac{6}{(n-3)(p''')^{\frac{n-3}{2}}} + \frac{4}{(n-2)(p''')^{\frac{n-2}{2}}} + \frac{1}{(n-1)(p''')^{\frac{n-1}{2}}} \right],$$

$$\bar{J}_3(p) = 2 \left[\frac{1}{(n-5)p^{\frac{n-5}{2}}} - \frac{4}{(n-4)p^{\frac{n-4}{2}}} + \frac{6}{(n-3)p^{\frac{n-3}{2}}} - \frac{4}{(n-2)p^{\frac{n-2}{2}}} + \frac{1}{(n-1)p^{\frac{n-1}{2}}} \right]$$

By properly choosing p we can make the difference of the two extreme sides of the inequalities (3.9) and (3.14) as small as we like and then have approximately

(3.17)

$$\sum_n^{(0)} = \sum_{q=1}^{p-1} \frac{v_q^{(0)}}{q^{n/2}} + \bar{J}_1(p)$$

$$\sum_n^{(2)} = \sum_{q=1}^{p-1} \frac{v_q^{(2)}}{q^{n/2}} + \bar{J}_1(p)$$

If p is large enough, then quite a good approximation is obtained by considering only the first term of $\bar{J}_1(p)$; then we can write

(3.18)

$$\sum_n^{(0)} = \sum_{q=1}^{p-1} \frac{v_q^{(0)}}{q^{n/2}} + \frac{4\pi}{(n-3)p^{\frac{n-3}{2}}}$$

$$\sum_{n+4}^{(2)} = \sum_{q=1}^{p-1} \frac{v_q^{(2)}}{q^{\frac{n+4}{2}}} + \frac{4\pi}{5(n-3)p^{\frac{n-3}{2}}}$$

This consideration holds for the simple cubic lattice. For other two lattice types a small modification has to be applied namely this: While the simple lattice has one cell per particle, face centred has two and body centred four cells per particle. Therefore it is easily seen, that for the face centred and the body centred lattice the remainder sums of the infinite series are one half and one fourth of those of the simple lattice.

CHAPTER IV.

Calculations of the lattice sums — continued.

Using the well known formula

$$(4.1) \quad \Gamma\left(\frac{n}{2}\right) r^{-\frac{n}{2}} = \int_0^\infty e^{-r^2 u} u^{\frac{n}{2}-1} du$$

we have for any lattice sum of the form

$$(4.2) \quad S_n = \sum_L \frac{C_L}{(l_1^2 + l_2^2 + l_3^2)^{n/2}}$$

the integral representation

$$(4.3) \quad S_n = \frac{1}{\Gamma\left(\frac{n}{2}\right)} \int_0^\infty u^{\frac{n}{2}-1} \sigma(u) du$$

where

$$(4.4) \quad \sigma(u) = \sum_L C_L e^{-(l_1^2 + l_2^2 + l_3^2)u}$$

We apply this to our two types of lattice sums

A. For $S_A^{(0)}$, we have

$C_0 = 0$ and $C_L = 1$ for $L \neq 0$. l_1, l_2 and l_3 should not be simultaneously zero.

In case of simple lattice l_1, l_2 and l_3 have all possible positive and negative integral values.

Denoting $\sigma(u)$ for simple lattice, case A, by $\sigma_S^{(0)}(u)$

we get

$$(4.5) \quad \sigma_S^{(0)}(u) = \left(\sum_{p=0, \pm 1, \pm 2, \dots} e^{-p^2 u} \right)^3 - 1 = \mathcal{J}_3^3(0, e^{-u}) - 1$$

the term -1 being introduced to cancel the term $+1$ occurring in $\left(\sum_{p=0, \pm 1, \pm 2, \dots} e^{-p^2 u} \right)^3$ when $p=0$ in all the three

factors, the case to be excluded.

In body centred lattice, l_1, l_2, l_3 are all even or all odd, hence

$$(4.6) \quad \sigma_h^{(o)}(u) = \left(\sum_{p=0, \pm 2, \pm 4, \dots} e^{-p^2 u} \right)^3 + \left(\sum_{p=\pm 1, \pm 3, \pm 5, \dots} e^{-p^2 u} \right)^3 - 1$$

$$= \left(\sum_{\lambda=-\infty}^{\infty} e^{-4\lambda^2 u} \right)^3 + \left(\sum_{\lambda=-\infty}^{\infty} e^{-4(\lambda - \frac{1}{2})^2 u} \right)^3 - 1$$

so that

$$(4.6a) \quad \sigma_h^{(o)}(u) = \vartheta_3^3(0, e^{-4u}) + \vartheta_2^3(0, e^{-4u}) - 1$$

In face centred lattice, l_1, l_2, l_3 are all even or one even and two odd, hence

$$(4.7) \quad \sigma_f^{(o)}(u) = \left(\sum_{p=0, \pm 2, \pm 4, \dots} e^{-p^2 u} \right)^3 + 3 \sum_{p=0, \pm 2, \pm 4, \dots} e^{-p^2 u} \left(\sum_{p=\pm 1, \pm 3, \dots} e^{-p^2 u} \right)^2 - 1$$

so that

$$(4.7a) \quad \sigma_f^{(o)}(u) = \vartheta_3^3(0, e^{-4u}) + 3\vartheta_3(0, e^{-4u})\vartheta_2^2(0, e^{-4u}) - 1$$

B.

For $S_n^{(2)}$ we have

$C_0 = 0$, $C_l = l^4$ for $l \neq 0, l_1, l_2$ and l_3 not being simultaneously ~~not~~ zero.

We get quite easily

(4.8)

$$\sigma_s^{(2)}(u) = \vartheta_3^2(0, \bar{e}^u) \frac{\partial^2 \vartheta_3(0, \bar{e}^u)}{\partial u^2},$$

(4.9)

$$\sigma_h^{(2)}(u) = \vartheta_3^2(0, \bar{e}^{4u}) \frac{\partial^2 \vartheta_3(0, \bar{e}^{4u})}{\partial u^2} + \vartheta_2^2(0, \bar{e}^{4u}) \frac{\partial^2 \vartheta_2(0, \bar{e}^{4u})}{\partial u^2}$$

(4.10)

$$\begin{aligned} \sigma_f^{(2)}(u) = & \vartheta_3^2(0, \bar{e}^{4u}) \frac{\partial^2 \vartheta_3(0, \bar{e}^{4u})}{\partial u^2} + \vartheta_2^2(0, \bar{e}^{4u}) \frac{\partial^2 \vartheta_3(0, \bar{e}^{4u})}{\partial u^2} \\ & + 2 \vartheta_2(0, \bar{e}^{4u}) \vartheta_3(0, \bar{e}^{4u}) \frac{\partial^2 \vartheta_2(0, \bar{e}^{4u})}{\partial u^2}. \end{aligned}$$

Here the $\vartheta(0, q) = \vartheta(q)$ are the well known ϑ functions (see Whittaker and Watson (1933) p. 464) which can be represented by rapidly converging power series in q ; for instance

$$\begin{aligned} \vartheta_3(q) &= 1 + 2q + 2q^4 + 2q^9 + \dots \\ \vartheta_4(q) &= 1 - 2q + 2q^4 - 2q^9 + \dots \\ \vartheta_2(q) &= 2q^{\frac{1}{4}} + 2q^{\frac{9}{4}} + 2q^{\frac{25}{4}} + \dots \end{aligned}$$

They satisfy the following transformation laws

$$\begin{aligned} \vartheta_3(e^{-\pi/\beta}) &= \frac{1}{\sqrt{\beta}} \vartheta_3(e^{-\pi/\beta}) \\ \vartheta_4(e^{-\pi/\beta}) &= \frac{1}{\sqrt{\beta}} \vartheta_2(e^{-\pi/\beta}) \\ \vartheta_2(e^{-\pi/\beta}) &= \frac{1}{\sqrt{\beta}} \vartheta_4(e^{-\pi/\beta}) \end{aligned}$$

Using these we split the integrals (4.3) for S_λ in two rapidly converging parts; for instance we have for

SIMPLE LATTICE

$$(4.13) \quad \sum_n^{(0)} = \frac{1}{\Gamma(\frac{n}{2})} \int_0^\infty u^{\frac{n}{2}-1} (\vartheta_3^3(\bar{e}^{-u}) - 1) du.$$

Putting $\frac{n}{2} - 1 = m$ and $u = \pi\beta$, we

get

$$\begin{aligned}
 \int_{\pi}^{(0)} &= \frac{\pi^{m+1}}{\Gamma(m+1)} \int_0^{\infty} \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta \\
 (4.14) \quad &= \frac{\pi^{m+1}}{\Gamma(m+1)} \mathcal{J}_m^{(0)}
 \end{aligned}$$

where

$$\begin{aligned}
 \mathcal{J}_m^{(0)} &= \int_0^{\infty} \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta \\
 (4.15) \quad &= \int_1^{\infty} \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta + \int_0^1 \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta.
 \end{aligned}$$

In the second integral we use the \mathcal{Q} transformation by which that interval also becomes $1 \leq \beta \leq \infty$.

Putting $\beta = \frac{1}{\gamma}$ we get

$$\begin{aligned}
 \int_0^1 \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta &= \int_1^{\infty} \frac{1}{\gamma^{m+1}} \mathcal{J}_3^3(e^{-\pi/\gamma}) d\gamma - \int_0^1 \beta^m d\beta \\
 (4.16) \quad &= \int_1^{\infty} \frac{1}{\gamma^{m+\frac{1}{2}}} \mathcal{J}_3^3(e^{-\pi/\gamma}) d\gamma - \frac{1}{m+1},
 \end{aligned}$$

so that

$$\mathcal{J}_m^{(0)} = \int_1^{\infty} \beta^m \left(\mathcal{J}_3^3(e^{-\pi\beta}) - 1 \right) d\beta + \int_1^{\infty} \frac{\mathcal{J}_3^3(e^{-\pi/\gamma}) d\gamma}{\beta^{m+\frac{1}{2}}} - \frac{1}{m+1}.$$

(4.17)

Here we use the power series (4.11) for $\mathcal{J}_3(q)$ and introduce

$$\mathcal{J}_3^3(q) = 1 + 6q + 12q^2 + 8q^3 + 6q^4 + \dots$$

(4.18)

Then we integrate term by term. We find that we have to evaluate an integral of the type

$\int_1^{\infty} \beta^m e^{-\beta x} d\beta$. We introduce a new function ϕ and put

(4.19)

$$\phi_m(x) = \int_1^{\infty} \beta^m e^{-\beta x} d\beta$$

where m may have the values $0, \pm \frac{1}{2}, \pm 1, \pm \frac{3}{2}, \pm 2, \dots$
 and $x = \frac{\beta\pi}{4}$ for $\beta = 0, \pm 1, \pm 2, \dots$

Integrating by parts we get

$$\begin{aligned} \phi_m(x) &= \left[\frac{e^{-\beta x}}{-x} \beta^m \right]_1^{\infty} - \int_1^{\infty} \frac{e^{-\beta x}}{-x} m \beta^{m-1} d\beta \\ &= \frac{e^{-x}}{x} + \frac{m}{x} \int_1^{\infty} e^{-\beta x} \beta^{m-1} d\beta \end{aligned}$$

so that $\phi_m(x)$ satisfy the recurrence formula

(4.20)

$$\phi_m(x) = \frac{e^{-x}}{x} + \frac{m}{x} \phi_{m-1}(x)$$

Now

$$\phi_0(x) = \int_1^{\infty} e^{-\beta x} d\beta = \frac{e^{-x}}{x}$$

$$\phi_{-\frac{1}{2}}(x) = \int_1^{\infty} e^{-\beta x} \beta^{-\frac{1}{2}} d\beta = 2 \int_1^{\infty} e^{-\alpha^2 x} d\alpha, \beta = \alpha^2$$

and putting $\alpha^2 x = y^2$ we get

$$\phi_{-\frac{1}{2}}(x) = \frac{2}{\sqrt{x}} \int_{\sqrt{x}}^{\infty} e^{-y^2} dy = \frac{\sqrt{\pi}}{\sqrt{x}} (1 - \Phi(\sqrt{x})) ;$$

$\Phi(x)$ is Gauss' error function, and is tabulated,
 (Burgess (7)).

And

$$\phi_{-1}(x) = \int_1^{\infty} \frac{e^{-x\beta}}{\beta} d\beta = \int_x^{\infty} \frac{e^{-\gamma}}{\gamma} d\gamma$$

(by putting $x\beta = \gamma$)

$$= -Ei(-x)$$

The function $Ei(x)$ is logarithmic integral (see Jahnke-Emde (12)) and is also tabulated, (Br. Ass. Adv. Sc. Math. Tab. Vol I (5)).

From the three functions

$$(4.21) \quad \begin{aligned} \phi_0(x) &= \frac{e^{-x}}{x} \\ \phi_{-\frac{1}{2}}(x) &= \frac{\sqrt{\pi}}{\sqrt{x}} \left(1 - \mathcal{E}(\sqrt{x}) \right) \\ \phi_{-1}(x) &= -Ei(-x) \end{aligned}$$

one can get all the $\phi_m(x)$ for different values of m with ^{the} help of the recurrence formula (4.20). Now as the published tables of the error integral and the logarithmic integral give values of the functions for one, two or at the most three decimal places of the argument, I had to interpolate for obtaining functions correct to eight, nine or even ten places of decimals by taking the argument correct to sixth or seventh decimal place. I have employed throughout my work Everett's Interpolation Formula (17) using second, fourth or sometimes even sixth central

differences. Then after obtaining the functions (4.21) for various values of x , tables IV have been completed for various values of m by using (4.20).

We go back to equation (4.17).

Using (4.18) we write (4.17) thus:

$$(4.22) \quad S_m^{(0)} = \int_1^\infty \beta^m \left((1 + 6e^{-\pi/\beta} + 12e^{-2\pi/\beta} + 8e^{-3\pi/\beta} + 6e^{-4\pi/\beta} + \dots) \right. \\ \left. + \int_1^\infty \frac{(1 + 6e^{-\pi/\beta} + 12e^{-2\pi/\beta} + 8e^{-3\pi/\beta} + 6e^{-4\pi/\beta} + \dots)}{\beta^{m+\frac{1}{2}}} d\beta \right) \\ - \frac{1}{m+1}.$$

The first term of the second integral imposes a condition on m and that is $m + \frac{1}{2} > 1$; this leads to $n \geq 4$. Using (4.19) we have

$$(4.23) \quad S_m^{(0)} = -\frac{1}{m+1} + 6\phi_m(\pi) + 12\phi_m(2\pi) + 8\phi_m(3\pi) + 6\phi_m(4\pi) \\ + \dots + \frac{1}{m-\frac{1}{2}} + 6\phi_{m-\frac{1}{2}}(\pi) + 12\phi_{m-\frac{1}{2}}(2\pi) + 8\phi_{m-\frac{1}{2}}(3\pi) + 6\phi_{m-\frac{1}{2}}(4\pi) + \dots$$

Now tables of ϕ functions being ready,

$S_m^{(0)}$ is easily obtained. Then equation (4.14) gives straight away the lattice sum $S_n^{(0)}$.

This method can be applied to all three lattice types and to both kinds of lattice sums.

BODY CENTRED LATTICE.

From (4.6a) and (4.3) we have

$$(4.24) \quad S_n^{(0)} = \frac{1}{\Gamma(\frac{n}{2})} \int_0^\infty u^{\frac{n}{2}-1} \left\{ \sqrt{\frac{3}{2}} (e^{-4u}) + \sqrt{\frac{2}{3}} (e^{-4u}) - 1 \right\} du.$$

Putting $\frac{n}{2} - 1 = m$, and $4u = \pi\beta$, we

get

$$(4.25) \quad S_n^{(0)} = \frac{\pi^{m+1}}{\Gamma(m+1)} S_m^{(0)},$$

where

$$\begin{aligned}
 (4.26) \quad J_m^{(0)} &= \frac{1}{4^{m+1}} \int_0^\infty \beta^m \left\{ \vartheta_3^3(e^{-\pi\beta}) + \vartheta_2^3(e^{-\pi\beta}) - 1 \right\} d\beta \\
 &= \frac{1}{4^{m+1}} \left[\int_1^\infty \beta^m \left\{ \vartheta_3^3(e^{-\pi\beta}) - 1 + \vartheta_2^3(e^{-\pi\beta}) \right\} d\beta \right. \\
 &\quad \left. + \int_1^\infty \frac{\vartheta_3^3(e^{-\pi\beta}) + \vartheta_4^3(e^{-\pi\beta})}{\beta^{m+\frac{1}{2}}} d\beta - \frac{1}{m+1} \right].
 \end{aligned}$$

The second line is due to the integration in the interval 0 to 1, the second integral being obtained by transformation equations (4.12).

Now

$$(4.27) \quad \vartheta_2^3(e^{-\pi\beta}) = 8 \left(e^{-\frac{3\pi\beta}{4}} + 3e^{-\frac{11\pi\beta}{4}} + \dots \right)$$

and

$$(4.28) \quad \vartheta_4^3(e^{-\pi\beta}) = 1 - 6e^{-\pi\beta} + 12e^{-2\pi\beta} - 8e^{-3\pi\beta} + 6e^{-4\pi\beta} - \dots$$

Substituting these values in (4.26) and expressing the integrals in terms of ϕ we get

$$\begin{aligned}
 (4.29) \quad J_m^{(0)} &= \frac{1}{4^{m+1}} \left[-\frac{1}{m+1} + \frac{4}{2m-1} + \sum_k a_k \phi_m(k\pi) \right. \\
 &\quad \left. + \sum_k b_k \phi_{m-\frac{1}{2}}(k\pi) + 8 \sum_k c_k \phi_m\left((k-\frac{1}{4})\pi\right) \right],
 \end{aligned}$$

the coefficients a_k , b_k and c_k being obtained from the following table:

k	a_k	b_k	c_k
1	6	0	1
2	12	12	0
3	8	0	3
4	6	6	0
5	.	.	.
-	-	-	-

FACE CENTRED LATTICE.

From (4.7a) and (4.3) we have

$$(4.30) \quad S_n^{(0)} = \frac{1}{\Gamma(\frac{n}{2})} \int_0^\infty u^{\frac{n}{2}-1} \left\{ \mathcal{J}_3^3(e^{-4u}) + 3\mathcal{J}_3(e^{-4u}) \mathcal{J}_2^2(e^{-4u}) - 1 \right\} du.$$

Proceeding as in body centred lattice we get

$$S_n^{(0)} = \frac{\pi^{m+1}}{\Gamma(m+1)} J_m^{(0)}$$

where

$$(4.31) \quad J_m^{(0)} = \frac{1}{4^{m+1}} \left[-\frac{1}{m+1} + \frac{8}{2m-1} + \sum_k a_k \phi_m(k\pi) + 8 \sum_k b_k \phi_m(k\pi) + 12 \sum_k c_k \phi_m((k-\frac{1}{2})\pi) \right],$$

the table of coefficients being

k	a_k	b_k	c_k
1	6	0	1
2	12	0	2
3	8	4	2
4	6	3	4
5	.	.	.
-	-	-	-

In case B i.e. for $S_n^{(2)}$, we have to do a little more calculation and that is essentially due to the occurrence of the derivatives of ϑ functions. Let us consider first the simple lattice ,

SIMPLE LATTICE.

From (4.8) and (4.3) we have

$$(4.32) \quad S_n^{(2)} = \frac{1}{\Gamma(\frac{n}{2})} \int_0^\infty u^{\frac{n}{2}-1} \vartheta_3^2(e^{-u}) \frac{\partial^2 \vartheta_3(e^{-u})}{\partial u^2} du$$

Putting as before $\frac{n}{2}-1 = m$ and $u = \pi\beta$ we get

$$(4.33) \quad S_n^{(2)} = \frac{\pi^{m-1}}{\Gamma(m+1)} \vartheta_m^{(2)}$$

where

$$(4.34) \quad \vartheta_m^{(2)} = \int_0^\infty \beta^m \vartheta_3^2(e^{-\pi\beta}) \frac{\partial^2 \vartheta_3(e^{-\pi\beta})}{\partial \beta^2} d\beta$$

We break up the integral as suggested before in two parts, first being the integral from 0 to 1 and the second from 1 to ∞ . The latter is easy to handle. In the former let us consider the second derivative term,

$$\frac{\partial^2 \vartheta_3(e^{-\pi\beta})}{\partial \beta^2}$$

which by transformation

$$= \frac{\partial^2}{\partial \beta^2} \left(\frac{1}{\sqrt{\beta}} \vartheta_3(e^{-\pi/\beta}) \right)$$

$$\begin{aligned}
&= \frac{\partial}{\partial \beta} \left[-\frac{1}{2\beta^{3/2}} \mathcal{J}_3(e^{-\pi/\beta}) + \frac{1}{\beta^{1/2}} \mathcal{J}_3'(e^{-\pi/\beta}) e^{-\pi/\beta} \frac{\pi}{\beta^2} \right] \\
&= \frac{\partial}{\partial \beta} \left[-\frac{1}{2\beta^{3/2}} \mathcal{J}_3(e^{-\pi/\beta}) + \frac{\pi}{\beta^{5/2}} e^{-\pi/\beta} \mathcal{J}_3'(e^{-\pi/\beta}) \right]
\end{aligned}$$

(dashes denoting differentiations with respect to the argument $e^{-\pi/\beta}$),

$$\begin{aligned}
&= \frac{3}{4\beta^{5/2}} \mathcal{J}_3(e^{-\pi/\beta}) - \frac{\pi}{2\beta^{7/2}} e^{-\pi/\beta} \mathcal{J}_3'(e^{-\pi/\beta}) - \frac{5}{2} \frac{\pi}{\beta^{7/2}} e^{-\pi/\beta} \mathcal{J}_3'(e^{-\pi/\beta}) \\
&\quad + \frac{\pi}{\beta^{5/2}} e^{-\pi/\beta} \frac{\pi}{\beta^2} [\mathcal{J}_3'(e^{-\pi/\beta}) + e^{-\pi/\beta} \mathcal{J}_3''(e^{-\pi/\beta})] \\
&= \frac{3}{4\beta^{5/2}} \mathcal{J}_3(e^{-\pi/\beta}) - \frac{\pi}{\beta^{7/2}} e^{-\pi/\beta} \mathcal{J}_3'(e^{-\pi/\beta}) (3 - \frac{\pi}{\beta}) \\
&\quad + \frac{\pi^2}{\beta^{9/2}} e^{-\pi/\beta} \mathcal{J}_3''(e^{-\pi/\beta}).
\end{aligned}$$

Let us now consider the integral

$$\int_0^1 \beta^m \mathcal{J}_3^2(e^{-\pi/\beta}) \frac{\partial^2 \mathcal{J}_3(e^{-\pi/\beta})}{\partial \beta^2} d\beta;$$

for $\mathcal{J}_3^2(e^{-\pi/\beta})$ we put $\frac{1}{\beta} \mathcal{J}_3^2(e^{-\pi/\beta})$ and for the derivative we substitute (4.35); then we transform as in (4.16) so that the range of integration becomes

$1 \leq \beta \leq \infty$; thus we finally get for the integral the expression

$$\begin{aligned}
(4.36) \quad \int_1^\infty &\left(\frac{3}{4} \frac{\mathcal{J}_3^3(e^{-\pi/\beta})}{\beta^{m-\frac{3}{2}}} - \frac{3\pi}{\beta^{m-\frac{5}{2}}} \mathcal{J}_3^2 \mathcal{J}_3' + \frac{\pi^2 e^{-\pi/\beta}}{\beta^{m-\frac{7}{2}}} \mathcal{J}_3^2 \mathcal{J}_3' \right. \\
&\quad \left. + \frac{\pi^2}{\beta^{m-\frac{7}{2}}} e^{-\pi/\beta} \mathcal{J}_3^2 \mathcal{J}_3'' \right) d\beta,
\end{aligned}$$

dashes denoting differentiations with respect to the argument $e^{-\pi/\beta}$.

If to this we add

$$\int_1^{\infty} \beta^m \vartheta_3^2(e^{-\pi\beta}) \frac{\partial^2 \vartheta_3(e^{-\pi\beta})}{\partial \beta^2} d\beta$$

we get $\mathcal{S}_m^{(2)}$.

Now for ϑ_3 , ϑ_3' and ϑ_3'' we introduce the corresponding rapidly convergent series; then taking help of the ϕ functions we obtain

$$(4.37) \quad \mathcal{S}_m^{(2)} = \frac{3}{2(2m-5)} + 2\pi^2 \sum_k a_k \phi_m(k\pi) + \frac{3}{4} \sum_k b_k \phi_{-m+\frac{3}{2}}(k\pi) - 6\pi \sum_k c_k \phi_{-m+\frac{5}{2}}(k\pi) + 2\pi^2 \sum_k d_k \phi_{-m+\frac{7}{2}}(k\pi),$$

the coefficients a , b etc being collected in the following table:

k	a_k	b_k	c_k	d_k
1	1	6	1	1
2	4	12	4	4
3	4	8	4	4
4	16	6	4	16
5

Substituting the value of $\mathcal{S}_m^{(2)}$ in (4.33) we finally get the required sum $S_n^{(2)}$.

BODY CENTRED LATTICE.

By combining (4.3) with (4.9) we get

$$(4.38) \quad S_n^{(2)} = \frac{1}{\Gamma(\frac{n}{2})} \int_0^{\infty} u^{\frac{n}{2}-1} \left(\vartheta_3^2(e^{-4u}) \frac{\partial^2 \vartheta_3(e^{-4u})}{\partial u^2} + \vartheta_2^2(e^{-4u}) \frac{\partial^2 \vartheta_2(e^{-4u})}{\partial u^2} \right) du.$$

Putting $\frac{n}{2} - 1 = m$, and $4u = \pi\beta$ as we did ⁱⁿ (4.24) we obtain

$$(4.39) \quad S_n^{(2)} = \frac{\pi^{m-1}}{\Gamma(m+1)} J_m^{(2)}$$

with

$$(4.40) \quad J_m^{(2)} = \frac{1}{4^{m-1}} \int_0^\infty \beta^m \left\{ J_3^2(e^{-\pi\beta}) \frac{\partial^2 J_3(e^{-\pi\beta})}{\partial \beta^2} + J_2^2(e^{-\pi\beta}) \frac{\partial^2 J_2(e^{-\pi\beta})}{\partial \beta^2} \right\} d\beta.$$

Now as

$$J_2(e^{-\pi\beta}) = \frac{1}{\sqrt{\beta}} J_4(e^{-\pi/\beta}),$$

we easily see that

$$(4.41) \quad \frac{\partial^2 J_2(e^{-\pi\beta})}{\partial \beta^2} = \frac{3}{4\beta^{5/2}} J_4(e^{-\pi/\beta}) - \frac{\pi}{\beta^{7/2}} e^{-\pi/\beta} J_4'(e^{-\pi/\beta}) \left(3 - \frac{\pi}{\beta}\right) + \frac{\pi^2}{\beta^{9/2}} e^{-\frac{2\pi}{\beta}} J_4''(e^{-\pi/\beta}),$$

the right hand side being the same expressions as (4.35), with J_4 being substituted for J_3 . The rest of the calculation goes on as before i.e. as in the simple lattice. Thus we get

$$(4.42) \quad J_m^{(2)} = \frac{1}{4^{m-1}} \left[\frac{3}{2m-5} + 2\pi^2 \sum_k a_k \phi_m(k\pi) + \sum_k b_k \phi_{-m+\frac{3}{2}}(k\pi) - 48\pi \sum_k c_k \phi_{-m+\frac{5}{2}}(k\pi) + 16\pi^2 \sum_k d_k \phi_{-m+\frac{7}{2}}(k\pi) + \frac{\pi^2}{2} \sum_k e_k \phi_m((k-\frac{1}{4})\pi) \right],$$

with the following scheme of coefficients:-

k	a_k	b_k	c_k	d_k	e_k
1	1	0	0	0	1
2	4	12	1	1	0
3	4	0	0	0	83
4	16	6	1	4	0
5					

FACE CENTRED LATTICE.

Combining (4.3) with (4.10)

and proceeding as we did in the previous case we obtain

$$(4.43) \quad S_n^{(2)} = \frac{\pi^{n-1}}{\Gamma(n+1)} J_m^{(2)}$$

with

$$(4.44) \quad J_m^{(2)} = \frac{1}{4^{m-1}} \left[\frac{6}{2m-5} + 2\pi^2 \sum_k a_k \phi_m(k\pi) \right. \\ \left. + 24 \sum_k b_k \phi_{-m+\frac{3}{2}}(k\pi) - 96\pi \sum_k c_k \phi_{-m+\frac{5}{2}}(k\pi) \right. \\ \left. + 32\pi^2 \sum_k d_k \phi_{-m+\frac{7}{2}}(k\pi) + \frac{\pi^2}{2} \sum_k e_k \phi_m\left((k-\frac{1}{2})\pi\right) \right],$$

where the coefficients are as in the following table:-

k	a_k	b_k	c_k	d_k	e_k
1	1	0	0	0	1
2	4	0	0	0	18
3	4	4	1	1	82
4	16	3	1	4	196
5					

The thing that we need now is the table giving us ϕ'_2 for various arguments. We may just observe that as $m \geq 1$ we shall not require $\phi_m((k-\frac{1}{2})\pi)$ and $\phi_m((k-\frac{1}{4})\pi)$ for any negative suffixes, though of course we shall need $\phi_{\frac{1}{2}}(\pi)$ to calculate $\phi_m(\pi)$ for $m = \frac{3}{2}, \frac{5}{2}$ etc.

CHAPTER V.

TABLES.

In the previous chapter we have derived all the theoretical results which are necessary for our work and we can now proceed directly to obtaining the tables mentioned in Chapters III and IV. In the present chapter, I am giving bare tables suppressing all the numerical work.

TABLE I

p	l	m	n	$\nu_p^{(0)}$	$\nu_p^{(2)}$
1	1	0	0	6	2
2	1	1	0	12	8
3	1	1	1	8	8
4	2	0	0	6	32
5	2	1	0	24	136
6	2	1	1	24	144
7*	—	—	—	—	—
8	2	2	0	12	128
9	{	2	1	24	264
		3	0	6	162
10	3	1	0	24	656
11	3	1	1	24	664

* No number $4^a (8m + 7)$ is representable as the sum of three squares.

p	l	m	n	$\gamma_p^{(0)}$	$\gamma_p^{(2)}$
12	2	2	2	8	128
13	3	2	0	24	776
14	3	2	1	48	1568
15	—	—	—	—	—
16	4	0	0	6	512
17	{ 4	1	0	24	2056
	{ 3	2	2	24	904
18	{ 4	1	1	24	2064
	{ 3	3	0	12	648
19	3	3	1	24	1304
20	4	2	0	24	2176
21	4	2	1	48	4368
22	3	3	2	24	1424
23	—	—	—	—	—
24	4	2	2	24	2304
25	{ 4	3	0	24	2696
	{ 5	0	0	6	1250
26	{ 4	3	1	48	5408
	{ 5	1	0	24	5008
27	{ 3	3	3	8	648
	{ 5	1	1	24	5016
28	—	—	—	—	—
29	{ 4	3	2	48	5648
	{ 5	2	0	24	5128
30	5	2	1	48	10272
31	—	—	—	—	—
32	4	4	0	12	2048
33	{ 4	4	1	24	4104
	{ 5	2	2	24	5256

p	l	m	n	$\nu_p^{(0)}$	$\nu_p^{(2)}$
34	{4 5	3 3	3 0	24 24	3344 5648
35	5	3	1	48	11312
36	{4 6	4 0	2 0	24 6	4224 2592
37	6	1	0	24	10376
38	{5 6	3 1	2 1	48 24	11552 10384
39	—	—	—	—	—
40	6	2	0	24	10496
41	{4 5 6	4 4 2	3 0 1	24 24 48	4744 7048 21008
42	5	4	1	48	14112
43	5	3	3	24	6296
44	6	2	2	24	14464
45	{5 6	4 3	2 0	48 24	14352 11016
46	6	3	1	48	22048
47	—	—	—	—	—
48	4	4	4	8	2048
49	{7 6	0 3	0 2	6 48	4802 22288
50	{7 5 5	1 4 5	0 3 0	24 48 12	19224 15392 5000
51	{7 5	1 5	1 1	24 24	19224 10008
52	6	4	0	24	12416

p	l	m	n	$\nu_p^{(0)}$	$\nu_p^{(2)}$
53	{ 7 6	2 4	0 1	24 48	19336 24848
54	{ 7 5 6	2 5 3	1 2 3	48 24 24	38688 10128 11664
55	-	-	-	-	-
56	6	4	2	48	25088
57	{ 7 5	2 4	2 4	24 24	19464 9096
58	7	3	0	24	19856
59	{ 7 5	3 5	1 3	48 24	39728 10648
60	-	-	-	-	-

In this table $p = l_1^2 + l_2^2 + l_3^2 = l^2 + m^2 + n^2$
 and the relation between l_1, l_2, l_3 and l, m, n
 is as follows:-

	l_1	l_2	l_3
or	$\pm l$	$\pm m$	$\pm n$
or	$\pm l$	$\pm n$	$\pm m$
or	$\pm m$	$\pm l$	$\pm n$
or	$\pm m$	$\pm n$	$\pm l$
or	$\pm n$	$\pm l$	$\pm m$
or	$\pm n$	$\pm m$	$\pm l$

TABLE II

n	p	p'	p''	p'''
11	25	13	13	16
12	20	10	10	16
13	19	8	10	16
14	16	6	9	9
15	16	6	9	9

TABLE III

x	e^{-x}	$\Phi(\sqrt{x})$	$-Ei(-x)$
$\pi/2$.2078791	.9236808	
$3\pi/4$.0947802	.9700563	
π	.0432139	.9878109	.0109063
$3\pi/2$.0089833	.9978593	
2π	.0018674	.9996072	.00026042
$5\pi/2$.0003707	.999926088	
$11\pi/4$.00017699	.999967723	
3π	.000080698	.999985856	.000007803
$7\pi/2$.000016776	.9999972608	
4π	.000003487	.9999994646	.0000002583

TABLE IV.

	$x=\pi$	$x=2\pi$	$x=3\pi$	$x=4\pi$
$\phi_0(x)$.0137554	.0002972	.00000856	.00000028
$\phi_{\frac{1}{2}}(x)$.0156953	.0003192	.00000899	.00000029
$\phi_1(x)$.0181339	.0003445	.00000947	.00000030
$\phi_{\frac{3}{2}}(x)$.0212502	.0003734	.00000999	.00000031
$\phi_2(x)$.0252998	.0004069	.00001057	.00000033
$\phi_{\frac{5}{2}}(x)$.0306658	.0004458	.00001121	.00000034
$\phi_3(x)$.0379149	.0004915	.00001193	.00000036
$\phi_{\frac{7}{2}}(x)$.0479197	.0005455	.00001273	.00000038
$\phi_4(x)$.0620301	.0006101	.00001362	.00000040
$\phi_{\frac{9}{2}}(x)$.0823953	.0006879	.00001464	.00000042
$\phi_5(x)$.1124794	.0007827	.00001579	.00000044
$\phi_{\frac{11}{2}}(x)$.1580052	.0008994	.00001710	.00000046
$\phi_6(x)$.2286752	.0010446	.00001864	.00000049

TABLE V.

	$x = \pi$	$x = 2\pi$	$x = 3\pi$	$x = 4\pi$
$\phi_{-\frac{1}{2}}(x)$.0121890	.0002777	.00000817	.00000027
$\phi_{-1}(x)$.0109063	.0002604	.00000780	.00000026
$\phi_{-\frac{3}{2}}(x)$.0098421	.0002448	.00000747	.00000025
$\phi_{-2}(x)$.0089507	.0002313	.00000717	.00000024
$\phi_{-\frac{5}{2}}(x)$.0081961	.0002188	.00000689	.00000023
$\phi_{-3}(x)$.0075471	.0002070	.00000663	.00000022
$\phi_{-\frac{7}{2}}(x)$.0069861	.0001968	.00000640	.00000020
$\phi_{-4}(x)$.0065011	.0001880	.00000619	.00000019
$\phi_{-\frac{9}{2}}(x)$.0060761	.0001803	.00000600	.00000018

TABLE VI.

	$x = \frac{3\pi}{4}$	$x = \frac{11\pi}{4}$
$\phi_{\frac{1}{2}}(x)$.0345760	.00001946
$\phi_0(x)$.0402260	.00002049
$\phi_{\frac{1}{2}}(x)$.0475633	.00002162
$\phi_1(x)$.0572984	.00002286
$\phi_{\frac{3}{2}}(x)$.0705057	.00002424
$\phi_2(x)$.0888624	.00002574
$\phi_{\frac{5}{2}}(x)$.1150349	.00002750
$\phi_3(x)$.1533691	.00002943
$\phi_{\frac{7}{2}}(x)$.2111041	.00003163
$\phi_4(x)$.3005934	.00003412
$\phi_{\frac{9}{2}}(x)$.4434051	.00003696
$\phi_5(x)$.6781050	.00004024
$\phi_{\frac{11}{2}}(x)$	1.0752543	.00004408
$\phi_6(x)$	1.7670061	.00004844

These functions are used only for
body centred lattice sums.

TABLE VII.

	$x=\pi/2$	$x=3\pi/2$	$x=5\pi/2$	$x=7\pi/2$
$\phi_{1/2}(x)$.1079317	.0017479	.00004674	.00000146
$\phi_0(x)$.1323399	.0019063	.00004720	.00000152
$\phi_{1/2}(x)$.1666956	.0020918	.00005017	.00000159
$\phi_1(x)$.2165919	.0023108	.00005321	.00000166
$\phi_{3/2}(x)$.2915225	.0025722	.00005678	.00000174
$\phi_2(x)$.4081133	.0028871	.00006075	.00000183
$\phi_{5/2}(x)$.5963124	.0032709	.00006527	.00000192
$\phi_3(x)$.9117789	.0037443	.00007040	.00000202
$\phi_{7/2}(x)$	1.4610249	.0043357	.00007628	.00000213
$\phi_4(x)$	2.4541659	.0050846	.00008305	.00000226
$\phi_{9/2}(x)$	4.3178680	.0060466	.00009090	.00000240
$\phi_5(x)$	7.9441927	.0073012	.00010007	.00000255
$\phi_{11/2}(x)$	15.2509609	.0089635	.00011085	.00000272
$\phi_6(x)$	30.4769212	.0112025	.00012364	.00000292

These functions are used only for face centred lattice sums.

CHAPTER VI.

Results.

I have given in chapter V all those tables that are needed for obtaining the sums $S_n^{(0)}$ and $S_{n+4}^{(2)}$ by the two methods described in Chapter III and Chapter IV. I have obtained these two sums for the three different types of cubic lattices and collected them in table VIII. Then applying equations (2.6) and (2.7) I have calculated $A(n)$ and $B(n)$ and these are given in table IX. The last decimal given is correct.

The results are also represented by curves (plates I-III). One immediately sees that for the face centred lattice both $A(n)$ and $B(n)$ are monotone increasing from $n=4$ to 15. In the case of the body centred lattice $B(n)$ increases through the whole interval but $A(n)$ only for the lower value of n i.e. for $n < 5$. To show the maximum clearly this part of the curve has been drawn in a larger scale. There is, therefore, a small range of stability for the lattices where both exponents are sufficiently small. For the simple lattice $A(n)$ is monotone increasing but $B(n)$ is monotone decreasing. As $B(n)$ is rather small compared with $A(n)$, I have also drawn it on a larger scale.

TABLE VIII.

n	SIMPLE		FACE CENTRED		BODY CENTRED	
	$S_n^{(0)}$	$S_{n+4}^{(2)}$	$S_n^{(0)}$	$S_{n+4}^{(2)}$	$S_n^{(0)}$	$S_{n+4}^{(2)}$
4	16.5323	3.9796	6.3346	1.1979	2.51541	.46986
5	10.3775	2.7859	2.9995	.5460	.94676	.16716
6	8.4019	2.4178	1.8067	.3204	.45383	.07636
7	7.4670	2.2497	1.1808	.2056	.23638	.03810
8	6.9458	2.1589	.80012	.13754	.12784	.01982
9	6.6289	2.1048	.55210	.09407	.07050	.01057
10	6.4261	2.0706	.38473	.06512	.03936	.00571
11	6.2923	2.0484	.26960	.04543	.02212	.00312
12	6.2021	2.0334	.18956	.03185	.01249	.00172
13	6.1406	2.0232	.13355	.02238	.007090	.000952
14	6.0982	2.0162	.09421	.01576	.004031	.000529
15	6.0688	2.0114	.06651	.01112	.002298	.000296

TABLE IX.

n	SIMPLE		FACE CENTRED		BODY CENTRED	
	A(n)	B(n)	A(n)	B(n)	A(n)	B(n)
4	3.50	.83	2.10	1.30	2.044	1.32
5	4.96	.68	2.23	1.59	2.062	1.65
6	6.36	.54	2.38	1.87	2.056	1.98
7	7.70	.43	2.55	2.15	2.029	2.32
8	8.98	.34	2.73	2.42	1.98	2.67
9	10.2	.26	2.93	2.68	1.92	3.02
10	11.4	.20	3.14	2.95	1.84	3.38
11	12.5	.15	3.35	3.22	1.75	3.75
12	13.7	.116	3.60	3.46	1.66	4.11
13	14.8	.088	3.82	3.73	1.56	4.48
14	15.8	.066	4.06	3.98	1.46	4.85
15	16.8	.050	4.28	4.24	1.36	5.22



PLATE 1

SIMPLE LATTICE

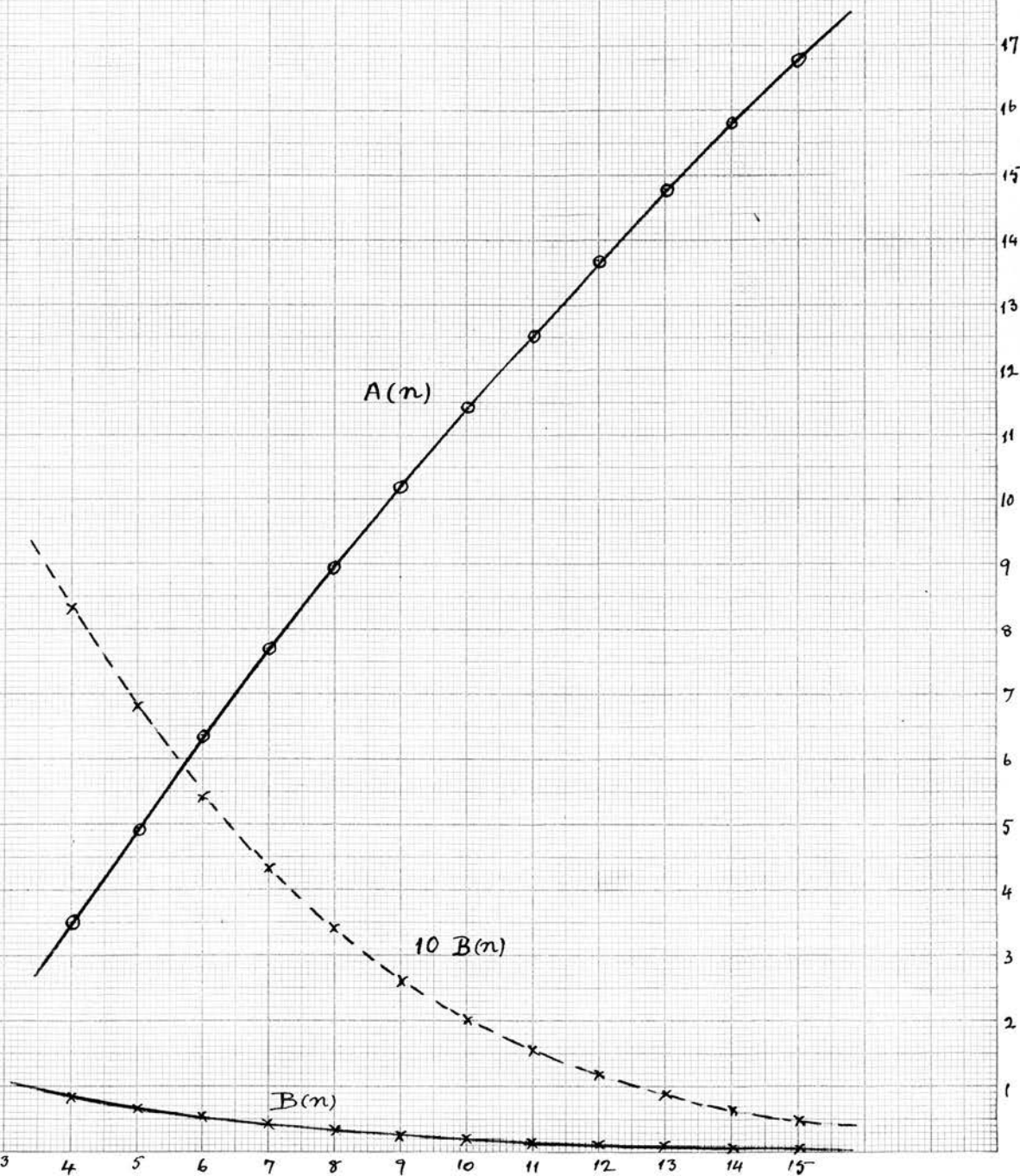
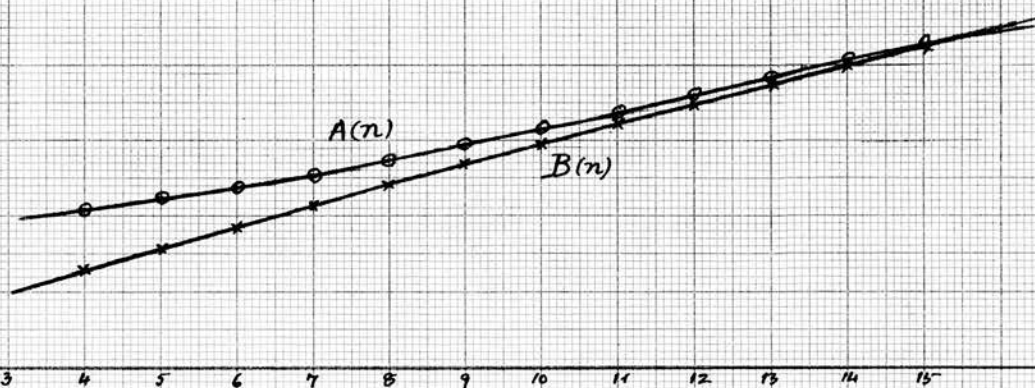
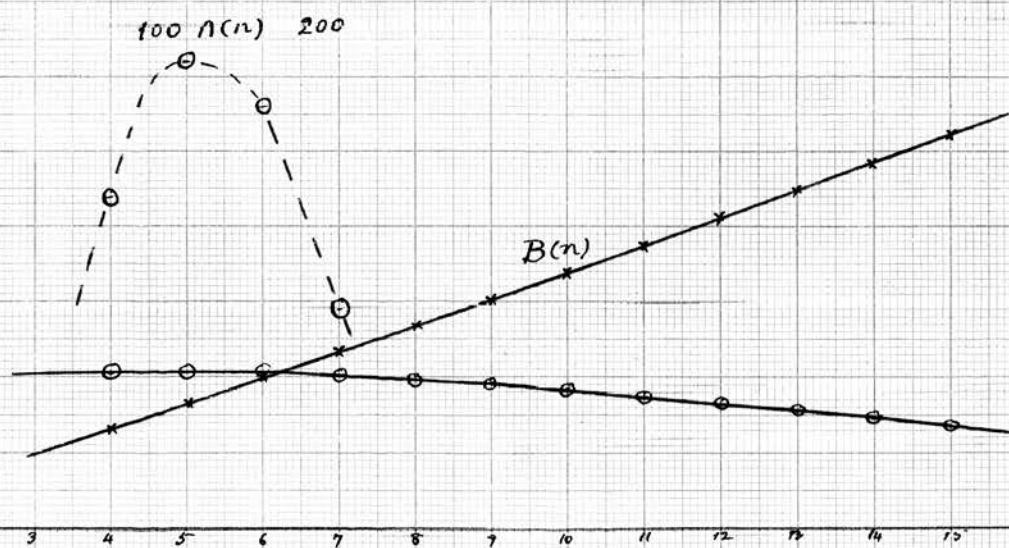


PLATE 2



FACE CENTRED LATTICE

PLATE 3



BODY CENTRED LATTICE

CONCLUSION.

Under the assumption that the potential energy of the three cubic lattices of the Bravais type consists of two terms, one attractive and proportional to r^{-m} and the other repulsive and proportional to r^{-n} , $n > m$ stability conditions could be expressed in the form that two functions of the number n are monotone increasing. When these functions are numerically worked out for $n = 4$ to 15 we find the face centred lattice to be the only one that is completely stable. Simple lattice is always unstable while the body centred is unstable for large exponents of the law of force.

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SUPPLEMENTARY PAPERS.

**ON HILBERT'S CURVE AND A NEW TYPE OF
NON-DIFFERENTIABLE FUNCTIONS.**

ON HILBERT'S CURVE AND A NEW TYPE OF
NON-DIFFERENTIABLE FUNCTIONS.*

INTRODUCTION

In the year 1891, Hilbert (4) defined geometrically a curve which passes through every point of a given area — a unit square (see figs. 1-4). The curve is obtained as the limit of a sequence of polygonal stretches. An analytical method of defining a parameter curve given by the equations of the form

$$x = \phi(t), \quad y = \psi(t)$$

and possessing the property of filling an area had already been given by Peano (7); and Moore (6) and Schoenflies (8) had subsequently developed a general geometrical method for defining space-filling curves. No analytical method of defining Hilbert's curve has been given so far. The object of the present paper is to supply such a definition.

It has been possible to define by the help of a parameter t two functions

$$x = f_1(t), \quad y = f_2(t)$$

* This is a combination of a published paper, "On Hilbert's curve", Proc. Benares Math Soc. 16 (1934), 13-34 and another unpublished paper "On a new type of non-differentiable function".

which define an (x,y) curve which fills the unit square. The functions $f_1(t)$ and $f_2(t)$ have been so chosen ~~so~~ that the analytically defined curve is the same as the curve defined by Hilbert.

It is found that the functions $f(t)$ are non-differentiable functions of t , and further that they are different from any non-differentiable functions defined by previous writers viz., Weierstrass (11), Darboux (2), Dini (3), Peano (7), Koch (5), Sierpinski (9), Singh (10), Bolzano (1) and others.

The functions are defined and the space-filling property of the curve proved in §1; in §2 is proved the continuity of the functions $f(t)$. That these functions are nowhere differentiable is shown in §3. The proof of the identity of the curve obtained by the analytical definition with that of Hilbert is given in §4.

§1.

Analytical Representations.

If $t = .a_1 a_2 a_3 \dots a_n \dots$ where the a 's are either 0 or 1 and the base of the radix fraction be 2, then t represents for different values of a 's all the points, rational and irrational, of the closed interval $(0,1)$.

The space-filling curve (x,y) which passes through all the points of a unit square is represented

by the functional equation

$$(1.1) \quad x = f_1(t) \quad , \quad y = f_2(t)$$

such that

$$(1.2) \quad x = .b_1 b_2 \dots b_m \dots$$

$$(1.3) \quad y = .c_1 c_2 \dots c_m \dots$$

where the b's and c's are individually either +1 or -1 depending upon the a's. The relationship between the a's, b's and c's is given below, the base of the radix fraction in the representation of the latter also being 2.

It may be noted here that t may be an irrational point or a rational one, represented by a non-ending sequence or an ending one, but the corresponding values of x and y are always represented by non-ending sequences in which no b's or c's are zero.

Certain particular notations are employed in the representations of x and y, they are the following:-

- (a) If a is an integer then $[a] = a$; if a is fractional lying between a' and a'' , then $[a] = a'$, $a' < a''$.
- (β) $\sigma_n = 1 + \left[\frac{a_1 + a_2}{2} \right] + \dots + \left[\frac{a_{2n-5} + a_{2n-4}}{2} \right],$
- (γ) $A_{2n} = \begin{cases} 0 & \text{if } a_1 + a_2 + \dots + a_{2n-2} \text{ be even} \\ a_{2n} & \text{if } a_1 + a_2 + \dots + a_{2n-2} \text{ be odd.} \end{cases}$

With the help of the above notations we now define*

$$\begin{aligned} b_1 &= 1 \\ (1.4) \quad b_{2m} &= (-)^{\sigma_{2m} + a_{4m-3} + A_{4m-1}} \\ b_{2m+1} &= (-)^{\sigma_{2m+1} + a_{4m-1} + a_{4m} - A_{4m}} \end{aligned}$$

and

$$\begin{aligned} c_1 &= 1 \\ (1.5) \quad c_{2m} &= (-)^{\sigma_{2m} + a_{4m-3} + a_{4m-1} - A_{4m-1}} \\ c_{2m+1} &= (-)^{\sigma_{2m+1} + a_{4m-1} + A_{4m}} \end{aligned}$$

For fixity of ideas, some particular cases are considered here .

Let

$$(1.6) \quad t = \frac{1}{2} + \frac{1}{2^2} + \frac{0}{2^3} + \frac{0}{2^4} + \dots$$

subsequent fractions being with zero numerators, i.e.

$$a_1 = 1, \quad a_2 = 1, \quad a_3 = a_4 = \dots = 0.$$

Substituting these values in (α) , (β) and (γ)

we get

$$\sigma_2 = 1, \quad \sigma_3 = \sigma_4 = \dots = 2$$

$$A_2 = A_4 = \dots = 0$$

$$b_2 = (-)^{1+1+0} = 1$$

$$b_3 = (-)^{2+0+0-0} = 1$$

* These definitions are the same as in my previously published paper "On Hilbert's Curve", but the notation is slightly different. This notation leads to much brevity.

and all the following b's are all equal to unity .

Similarly

$$c_2 = (-)^{1+1+1-0} = -1$$

$$c_3 = (-)^{2+0+0} = 1$$

and subsequent c's are all +1.

Thus

$$(1.7) \quad x = \frac{1}{2} + \frac{1}{2^2} + \frac{1}{2^3} + \dots + \frac{1}{2^n} + \dots \text{ to infinity} \\ = 1$$

and

$$(1.8) \quad y = \frac{1}{2} - \frac{1}{2^2} + \frac{1}{2^3} + \frac{1}{2^4} \dots + \frac{1}{2^n} + \dots \text{ to infinity} \\ = \frac{1}{2}$$

Another representation of the same t is

$$(1.9) \quad t = \frac{1}{2} + \frac{0}{2^2} + \frac{1}{2^3} + \frac{1}{2^4} + \dots + \frac{1}{2^n} + \dots$$

Here $a'_1 = 1$, $a'_2 = 0$, $a'_3 = a'_4 = \dots = 1$.

Then

$$\sigma'_2 = 1,$$

$$\sigma'_3 = 1 + \left[\frac{0+1}{2} \right] = 1$$

$$\sigma'_4 = 2, \quad \sigma'_5 = 3,$$

$$\sigma'_n = n - 2, \quad n > 2$$

And

$$A'_2 = 0,$$

$$A'_4 = A'_6 = A'_8 = \dots = 1$$

Substituting these values in (1.4) and (1.5) we get

$$b'_2 = b'_4 = b'_6 = \dots = 1$$

$$b'_3 = b'_5 = \dots = 1$$

and

$$c'_2 = 1, \\ c'_3 = c'_4 = \dots = -1$$

Thus

$$(1.10) \quad x' = \frac{1}{2} + \frac{1}{2^2} + \dots + \frac{1}{2^n} + \dots \\ = 1$$

$$(1.11) \quad y' = \frac{1}{2} + \frac{1}{2^2} - \frac{1}{2^3} - \frac{1}{2^4} - \dots - \frac{1}{2^n} - \dots \\ = \frac{1}{2}$$

We therefore find that both the representations of t give the same values of x and y though in different sequences.

Let us now consider the general case.

If t is ^{an} irrational number, it will have a unique representation in terms of the fraction series; hence a 's being uniquely determined b 's and c 's will also be uniquely determined.

But if t is rational, it will have double representation and two cases will arise:

$$(1.12) \quad \text{Case A} \quad \begin{cases} t = . a_1 a_2 \dots a_{2m} 1 0 0 \dots 0 \dots \\ t' = . a_1 a_2 \dots a_{2m} 0 1 1 \dots 1 \dots \end{cases}$$

$$(1.13) \quad \text{Case B} \quad \begin{cases} t = . a_1 a_2 \dots a_{2m} a_{2m+1} 1 0 0 \dots 0 \dots \\ t' = . a_1 a_2 \dots a_{2m} a_{2m+1} 0 1 1 \dots 1 \dots \end{cases}$$

These two cases are different because of the unsymmetric definitions of A 's, b 's and c 's in terms of a_{2m} and a_{2m+1} .

It is obvious from the equations (β) and (γ) that in both the cases A and B, we have

$$(1.14) \quad \begin{cases} \sigma_2 = \sigma_2, \dots, \sigma_{m+2} = \sigma'_{m+2} \\ A_2 = A'_2, \dots, A_{2m} = A'_{2m}, \end{cases}$$

and therefore

$$(1.15) \quad \begin{cases} b_i = b'_i, \dots, b_{m+1} = b'_{m+1} \\ c_i = c'_i, \dots, c_{m+1} = c'_{m+1} \end{cases}$$

Let us now consider the two cases separately.

Case A. Let p be any positive integer. Combining (1.12) with (β) and (γ) we easily get

$$\begin{aligned} \sigma_{m+3} &= \sigma_{m+2+p} = \sigma_{m+2} \\ A_{2(m+1)} &= A_{2(m+1+p)} = 0 \\ \sigma'_{m+3} &= \sigma_{m+3} = \sigma_{m+2} \\ \sigma'_{m+2+p} &= \sigma_{m+2} + (p-1) \\ A'_{2(m+1)} &= 0, \quad A'_{2(m+1+p)} = 1 \text{ if } \sum_{p=1}^{2m} a_p \text{ is even} \end{aligned}$$

or

$$A'_{2(m+1)} = 1, \quad A'_{2(m+1+p)} = 0 \text{ if } \sum_{p=1}^{2m} a_p \text{ is odd.}$$

Substituting these values in (1.4) one observes immediately that b and b' are as follows:-

$\sum_{p=1}^{2m} a_p$	even				odd			
σ_{m+2}	even		odd		even		odd	
m	even	odd	even	odd	even	odd	even	odd
b_{m+2}	-1	-1	1	1	-1	-1	1	1
b'_{m+2}	1	-1	-1	1	-1	1	1	-1
b_{m+2+p}	1	1	-1	-1	1	1	-1	-1
b'_{m+2+p}	-1	1	1	-1	1	-1	-1	1

This table shows that b_{m+2+p} may or may not be equal to b'_{m+2+p} but x is always equal to x' , for the possible values of x are

$$(1.16) \quad x = .l_1, l_2, \dots, l_{m+1} \pm \frac{1}{2^{m+2}} \mp \frac{1}{2^{m+3}} \mp \frac{1}{2^{m+4}} \mp \dots$$

$$\text{i.e. } x = .l_1, l_2, \dots, l_{m+1} \quad \text{numerically;}$$

and the possible values of x are

$$(1.17) \quad x' = .l_1, l_2, \dots, l_{m+1} \pm \frac{1}{2^{m+2}} \mp \frac{1}{2^{m+3}} \mp \dots$$

$$\text{i.e. } x' = .l_1, l_2, \dots, l_{m+1} \quad \text{numerically.}$$

Case B.

In this case we have

$$\sigma_{m+3} = \sigma_{m+2+p} = \sigma_{m+2} + \left[\frac{a_{2m+1} + 1}{2} \right]$$

$$A_{2(m+1)} = 0 \text{ or } 1 \text{ according as } \sum_{p=1}^{2m} a_p \text{ is even or odd}$$

$$A_{2(m+1+p)} = 0$$

$$\sigma'_{m+3} = \sigma'_{m+1} = \sigma_{m+2}$$

$$\sigma'_{m+2+p} = \sigma_{m+2} + (p-1)$$

$$A'_{2(m+1)} = 0$$

$$A'_{2(m+1+p)} = 0 \text{ or } 1 \text{ according as } \sum_{p=1}^{2m+1} a \text{ is even or odd.}$$

Hence b and b' are as in the following table: -

$a_{2m+1} =$	0								1							
$\sum_{p=1}^{2m} a_p$	even				odd				even				odd			
σ_{m+2}	even		odd		even		odd		even		odd		even		odd	
m	even	odd	even	odd	even	odd	even	odd	even	odd	even	odd	even	odd	even	odd
b_{m+2}	1	-1	-1	1	-1	1	1	-1	-1	1	1	-1	1	-1	-1	1
b'_{m+2}	1	1	-1	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	1
b_{m+2+p}	1	1	-1	-1	1	1	-1	-1	-1	-1	1	1	-1	-1	1	1
b'_{m+2+p}	1	-1	-1	1	-1	1	1	-1	-1	1	1	-1	1	-1	-1	1

The table shows that in this case also $x = x'$.

Hence we conclude that

t may be rational or irrational there will be one and only one corresponding value for x.

One infers immediately that the same is true for y.

We now consider the inverse problem of finding out the a's when b's and c's are given.

It is easily seen that if only b's or only c's are given we cannot determine the a's.

By comparing (1.4) and (1.5) we obtain that if

$$(1.18) \quad b_{n+1} = c_{n+1} \quad \text{then } a_{2n} = 0$$

$$91.19) \quad b_{n+1} = -c_{n+1} \quad \text{then } a_{2n} = 1$$

This will give us all the a's with even suffixes.

To determine the a's with odd suffixes we observe that as b_n is either +1 or -1, we would know at once, whether the index of (-) in (1.4) is even or odd. And as any a is either zero or unity, we could easily determine all the a's in succession beginning from a_1 .

Here arises a question whether it will make any difference to the values of a's if we employ one or the other of the two representations when x or y or both have double representations and whether this will affect the corresponding t in any manner. The answer is in the affirmative.

Three cases arise:-

- (1) x and y both having unique representations ,
- (2) One of the two having double representation ,
- (3) x and y both having double representation .

Case (1) : Since x and y both have unique representations, there is no ambiguity and the determination of the a's will also be unique; hence there will be only one corresponding t.

Case (2) : Let x have double representation

$$x = . b_1 b_2 \dots b_{n+1} -1 . 1 . 1 \dots$$

$$x' = . b_1 b_2 \dots b_{n+1} 1 . -1 . -1 \dots$$

and

$$y = . c_1 c_2 \dots c_{n+1} \dots$$

Corresponding to either representation of x , a 's upto a_{1n} will be the same. But a_{1n+1} and successive a 's with even suffixes will obviously be different from the corresponding a 's. Further at no stage in y can the subsequent c 's be all the same number, because in that case y would have double representation; but in the case of x all the b 's subsequent to b_{n+1} are the same number either 1 or -1. Therefore from equations (1.18) and (1.19) we get that at no stage could all the a 's with even suffixes be the same number zero or one. Hence we see that the different representations of x will not only give different sequence of a 's but also different t 's.

Case (3): Let the double representations be

$$(1.20) \quad \begin{cases} x = . b_1 b_2 \dots b_{n+1} -1 . 1 . 1 \dots \\ x' = . b_1 b_2 \dots b_{n+1} 1 . -1 . -1 \dots \end{cases}$$

and

$$(1.21) \quad \begin{cases} y = . c_1 c_2 \dots c_{m+1} -1 . 1 . 1 \dots \\ y' = . c_1 c_2 \dots c_{m+1} 1 . -1 . -1 \dots \end{cases}$$

where m and n may or may not be equal.

It would not be difficult to see by taking one value of x with one value of y , that in general in the four

different combinations of x and y we shall get four different values of t . There is one special case when $m = n$. In this case we find that out of four sequences for t , two give the same value. Thus in this particular case we ^{would} obtain only three different values of t . Let us consider this case now.

Let

$$(1.22) \quad \begin{cases} x = . b_1 b_2 \dots b_{m+1} -1 . 1 . 1 \dots \\ y = . c_1 c_2 \dots c_{m+1} -1 . 1 . 1 \dots \end{cases}$$

Then

$$a_{2(m+1)} = a_{2(m+\beta)} = 0$$

and therefore also

$$A_{2(m+1)} = A_{2(m+\beta)} = 0; \quad \sigma_{m+2+\beta} = \sigma_{m+2}$$

Substituting these values in (1.4) we get

$$a_{2m+1} = 1, \text{ and } a_{2(m+\beta)+1} = 0 \quad \text{if } \sigma_{m+2} \text{ is even}$$

and

$$a_{2m+1} = 0, \quad a_{2(m+\beta)+1} = 1 \quad \text{if } \sigma_{m+2} \text{ is odd}$$

Therefore

$$(1.23) \quad t = . a_1 a_2 \dots a_{2m} 1 0 0 \dots 0 \dots \quad \text{if } \sigma_{m+2} \text{ is even}$$

or

$$(1.24) \quad t = . a_1 a_2 \dots a_{2m} 0 1 0 1 \dots \quad \text{if } \sigma_{m+2} \text{ is odd}$$

Let us now take

$$(1.25) \quad \begin{cases} x = . b_1 b_2 \dots b_{m+1} 1. -1. -1 \dots -1 \dots \\ y = . c_1 c_2 \dots c_{m+1} 1. -1. -1 \dots -1 \dots \end{cases}$$

This time again

$$a_{2(m+1)} = a_{2(m+\beta)} = 0$$

$$A_{2(m+1)} = A_{2(m+\beta)} = 0$$

$$\sigma_{m+2+\beta} = \sigma_{m+2}$$

But when we substitute these values in (1.4) we get different $a_{2(m+p)+1}$ on account of b_{m+2+p} being different from those in (1.22); we have

$$a_{2m+1} = 0, \quad a_{2(m+p)+1} = 1 \quad \text{if } \sigma_{m+2} \text{ is even,}$$

and

$$a_{2m+1} = 1, \quad a_{2(m+p)+1} = 0 \quad \text{if } \sigma_{m+2} \text{ is odd,}$$

giving us

$$(1.26) \quad t = . a_1 a_2 \dots a_{2m} 0 1 0 1 \dots \quad \text{if } \sigma_{m+2} \text{ is even}$$

or

$$(1.27) \quad t = . a_1 a_2 \dots a_{2m} 1 0 0 \dots \quad \text{if } \sigma_{m+2} \text{ is odd.}$$

These alternative values are obviously different from (1.23) and (1.24) obtained in the previous case.

In the third combination

$$(1.28) \quad \begin{cases} x = . b_1 b_2 \dots b_{m+1} . -1. 1. 1 \dots \\ y = . c_1 c_2 \dots c_{m+1} . 1. -1. -1 \dots \end{cases}$$

Here we shall have

$$a_{2(m+1)} = a_{2(m+p)} = 1$$

and other a 's will then be as follows:

$\sum_{p=1}^{2m} a_p$	even				odd			
σ_{m+2}	even		odd		even		odd	
m	even	odd	even	odd	even	odd	even	odd
a_{2m+1}	1	0	0	1	0	1	1	0
$a_{2(m+p)+1}$	0	1	1	0	1	0	0	1

Therefore

$$(1.29) \quad t = . a_1 a_2 \dots a_{2m} 1 1 0 1 0 1 \dots 0 1 \dots$$

or

$$(1.30) \quad t = . a_1 a_2 \dots a_{2m} 0 1 1 1 \dots 1 1 \dots$$

The fourth combination is

$$(1.31) \quad \begin{aligned} x &= . b_1 b_2 \dots b_{m+1} . 1 . -1 . -1 \dots \\ y &= . c_1 c_2 \dots c_{m+1} -1 . 1 . 1 \dots \end{aligned}$$

Here again we shall have

$$a_{2(m+1)} = a_{2(m+p)} = 1$$

and other a 's will be as in this table:-

$\sum_{p=1}^{2m} a_p$	even				odd			
σ_{m+1}	even		odd		even		odd	
m	even	odd	even	odd	even	odd	even	odd
a_{2m+1}	0	1	1	0	1	0	0	1
$a_{2(m+p)+1}$	1	0	0	1	0	1	1	0

so that

$$(1.32) \quad t = . a_1 a_2 \dots a_{2m} 0 1 1 \dots 1 1 \dots$$

or

$$(1.33) \quad t = . a_1 a_2 \dots a_{2m} 1 1 0 1 0 1 \dots 0 1 \dots$$

It is quite obvious now that t obtained from the third combination is definitely different from that obtained in the fourth combination; but one of them is equal to the t of either of the two combinations, first or second, for

$$(1.34) \quad t = . a_1 a_2 \dots a_{2m} 0 1 1 \dots 1 1 \dots$$

$$(1.35) \quad = t = . a_1 a_2 \dots a_{2m} 1 0 0 \dots 0 0 \dots$$

Thus we have shown that we get only three different t 's if $m = n$ in equations (1.20) and (1.24) which give double representations of x and y . We conclude then, that the curve given by $x = f_1(t)$ and $y = f_2(t)$ passes through every point of the unit square once, twice, thrice or four times

depending upon the nature of the point whose coordinates may have unique or double representation.

§ 2.

CONTINUITY OF THE FUNCTIONS $f(t)$.

It is easy to see that the functions $f_1(t)$ and $f_2(t)$ are continuous functions of t . For if we take two points t_1 and t_2 which are very near to each other differing in the $2m$ th term of the radix fraction then the corresponding x_1 and x_2 i.e. $f_1(t_1)$ and $f_1(t_2)$ do not differ up to $(m-1)$ th term. Hence the difference between $f_1(t_1)$ and $f_1(t_2)$ can be made as small as we please by making the difference between t_1 and t_2 suitably small which shows that $f_1(t)$ is a continuous function of t . The same argument shows that $f_2(t)$ is also a continuous function of t .

§ 3.

NON-DIFFERENTIABILITY OF THE FUNCTIONS $f(t)$.

We now proceed to show that the functions $f_1(t)$ and $f_2(t)$ are non-differentiable functions of t . Two cases arise:—

1. Non-differentiability at the set of points t with double representation,
2. Non-differentiability at the set of points with unique representation.

Case.1. Of the two representations of a point t , one will be ending and the other non-ending. Let ending one be

$$(3.1) \quad t = . a_1 a_2 \dots a_r 0 0 \dots$$

Let us for simplicity assume for the moment that m is odd $r < 2m$ and $\sum_{p=1}^r a_p$ is even. We have then

$$a_{2m} = 0, \quad a_{2m+p} = 0$$

and

$$\sigma_{m+1} = \sigma_{m+1+p}$$

and

$$A_{2m} = A_{2(m+p)} = 0$$

We further notice from (1.4) that every a_{4p} occurs explicitly in one of the equations giving b 's but a_{4p-2} do not occur explicitly in any of the equations (1.4) which give b 's in terms σ , a and A . And as all $a_{2(m+p)}$ are zeros, a change in any one $a_{2(m+p)}$ will affect neither σ 's nor A 's. Therefore it is obvious that an addition of $\frac{1}{2^{2m+4s}}$ (s being any non-negative integer) to t , i.e. changing a_{2m+4s} from 0 into 1 will affect none of the b 's. Thus if we take a sequence of values for $h_s = \frac{1}{2^{2m+4s}}$, s ranging from 0 to ∞ , then $x' - x$ will always be zero, and

$$(3.2) \quad \therefore \lim_{h_s \rightarrow 0} \frac{x' - x}{h_s} = 0$$

But if $\frac{1}{2^{2m+2+4s}}$ be added to t , σ 's and A 's will remain unchanged but as

$$(3.3) \quad b_{m+2+2s} = (-)^{\sigma_{m+2+2s} + a_{2m+1+4s} + a_{2m+2+4s} - A_{2m+2+4s}}$$

b'_{m+2+2s} will have the sign opposite to that of b_{m+2+2s} while all other b 's will remain unchanged.

And if we take the sequence $h'_s = \frac{1}{2^{2m+2+4s}}$, giving to s in succession the values as before, we get

$$\lim_{h'_s \rightarrow 0} \frac{x'' - x}{h'_s} = \lim_{s \rightarrow \infty} \frac{\frac{\pm 2}{2^{2m+2+4s}}}{\frac{1}{2^{2m+2+4s}}}$$

$= +\infty$ or $-\infty$ depend-

ing upon the a 's. If $\sum_{p=1}^r a_p$ be odd, then the first case gives the limit to be $+\infty$ or $-\infty$ while the second case gives zero.

If m be even then also, as one can easily see, the two limits will not only be different but also be 0 and $\pm\infty$.

These results prove that in Case 1 i.e. when t has double representation, the function $f_1(t)$ has no differential coefficient at t . Further more $f_1(t)$ has also no progressive derivate as the two sequences h_s and h'_s give different limits.

The case of $f_2(t)$ is similar to $f_1(t)$.

Case 2. As in this case ^{since} at no stage can the subsequent a 's be all 0 or all 1, the representation of t may belong to one of the following classes: -

(i) 0's and 1's are not arranged in any regular order.

(ii) The zero a 's are inserted between unit a 's satisfying certain conditions.

(iii) The unit a 's are inserted between zero a 's satisfying certain conditions.

We consider these classes one by one.

Class (1). From the analysis of Case 1 we easily see that if any a_{2m} be zero with m and $\sum_{p=1}^{2(m-1)} a_p$ odd then the addition of $\frac{1}{2^{2m}}$ to t changes a_{2m} from 0 to 1 and b_{m+1} from +1 to -1 (or from -1 to +1). All the b 's before b_{m+1} remain unaltered. Subsequent b 's may change but as they would not be all +1 or -1 so the change in the sign of b_{m+1} will bring about a change in the value of x . Thus $\frac{x'-x}{t'-t}$ will be large and positive or negative, this depending upon the value of b_{m+1} . Now as the zero a 's and unit a 's are not arranged in any regular order we can take a sequence $\frac{1}{2^{2m+4s}}$ for such values of s for which a_{2m+4s} is zero and $\sum_{p=1}^{2(m-1)+4s} a_p$ odd and further that the change in the sign of b_{m+1+2s} is always from +1 to -1 (or from -1 to +1) i.e. σ_{m+1+2s} is even (or odd); and

$\lim_{h_s \rightarrow 0} \frac{x' - x}{t' - t} = -\infty \text{ or } +\infty$ according

as b_{m+1} was originally +1 or -1.

Next we choose another sequence of $\frac{1}{2^{2n+4q}}$ satisfying the conditions that n and $\sum_{p=1}^{2(n-1)+4q} a_p$ are odd, but σ_{n+1+2q} is odd if σ_{m+1+2s} was even and vice-versa, so that b_{n+1+2q} changes sign from -1 to +1 if b_{m+1+2s} changed sign from +1 to -1 and vice-versa. We shall thus get

$$\lim_{h_q \rightarrow 0} \frac{x'' - x}{t'' - t} = +\infty \text{ or } -\infty$$

We have thus shown that by taking two different sequences h_s and h_q we get two different limits for the derivate. Therefore no progressive derivate

value exists for such values of t as belong to class (i).

Class (ii) There are two possibilities:-

First - Zeros may be arranged in such a manner that it is impossible to get two sequences h_s and h_r satisfying the conditions mentioned in class (i), i.e. no sequence h_q exists which may give the change in the value of b_{n+i+q} to be opposite in sign to the change of b_{m+s+i} .

Second - None of the a_{2m} 's are zeros. Some special cases will be considered here, those cases which may not be considered in the following pages can be treated by one or the other of the given methods.

First Case:

Let $t = . a_1 a_2 \dots a_{2m-1} . 0 . a_{2m+1} \dots a_{2n-1} . 0 . a_{2n+1} \dots$
 where $a_{2m-1} = 1$, a_{2m+1} and a 's upto a_{2n-1} are all 1;
 further let

m and $\sum_{p=1}^{2(m-1)} a_p$ be odd and σ_{m+1} even.

Then

$$A_{2m} = 0, A_{2(m+r)} = 0, m+r \leq n.$$

This gives

$$b_{m+1} = -1, b_{m+2} = +1 = b_{m+1+r}.$$

If we subtract $\frac{1}{2^{2m-1}}$ from t then a_{2m-1} becomes zero and $A'_{2m} = 0, A'_{2(m+r)} = 1$.

This gives

$$b'_{m+1} = 1, b'_{m+1+r} = -1$$

and

$$\frac{x' - x}{t' - t} = -2 \times 2^{2m-1} \left(\frac{1}{2^{m+1}} - \frac{1}{2^{m+2}} - \dots - \frac{1}{2^{m+n}} \right)$$

Hence taking a proper sequence of h_s we can easily get

$$\lim_{t' \rightarrow t} \frac{x' - x}{t' - t} = -\infty$$

If on the other hand we subtract $\frac{1}{2^{2m+1}}$, then a_{2m+1} becomes zero; $A''_{2m} = 0$, $A''_{2m+2} = 1$, $A''_{2(m+1+r)} = 0$, σ''_{m+2} and σ''_{m+3} are even; hence $b''_{m+1} = -1$, $b''_{m+2} = +1$, $b''_{m+3} = -1$, ... and by taking a suitable sequence h_s we can get

$$\lim_{t' \rightarrow t} \frac{x' - x}{t' - t} = +\infty$$

Hence we have shown that in such a case no regressive derivate exists.

It is not difficult to see that if the above conditions are not satisfied some other will be satisfied because of some regularity in the occurrence of zero and unit a 's and one can always select suitable sequences to show that either the progressive or the regressive derivate does not exist.

Second Case: This case can be treated in the same way as the first case.

Class (iii) Let most of the a 's be zero except a few a 's which are equal to 1.

$$\text{Let } t = .a_1 a_2 \dots a_{2m} 0 0 \dots 0 a_{2n} 0 \dots$$

where a_{2m} and a_{2n} are unity. As before for argument's sake let m and $\sum_{p=1}^{2(m-1)} a_p$ be odd and σ_{m+1} even. Then

$$A_{2m} = 1, \quad A_{2(m+r)} = 0, \quad m+r \leq n;$$

hence

$$b_{m+1} = -1, \quad b_{m+2} = 1 \geq b_{m+1+r}$$

Now if we add $\frac{1}{2^{2m+1}}$ to t , we make no alterations in the A 's and σ 's. Thus

$$b'_{m+1} = -1, \quad b'_{m+2} = -1, \quad b'_{m+3} = 1 \dots$$

And then choosing a suitable sequence of h_s we can get

$$\lim_{t' \rightarrow t} \frac{x' - x}{t' - t} = -\infty$$

But if we were to add $\frac{1}{2^{2m-1}} + \frac{1}{2^{2m+1}}$ we shall have σ_{m+2} odd, A 's remaining unchanged; hence

$$b''_{m+1} = 1, \quad b''_{m+2} = 1, \quad b''_{m+3} = -1, \dots$$

and choosing a suitable sequence for h'_s we can easily get

$$\lim_{t'' \rightarrow t} \frac{x'' - x}{t'' - t} = +\infty$$

Thus no progressive derivate exists.

We can similarly show in other cases too that either the progressive or the regressive derivate does not exist.

The significance of showing that either the progressive or the regressive derivate does not exist is that the function $f_1(t)$ is not only nowhere differentiable but also it has no cusps.

The case ^{of} $f_2(t)$ is similar to $f_1(t)$.

§ 4

Identity of this curve with Hilbert's curve.

It has already been stated

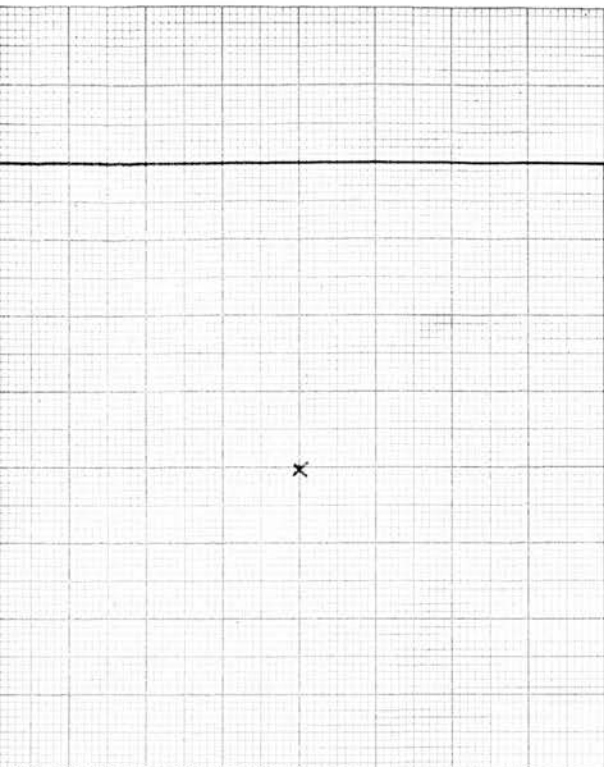


FIG. 1

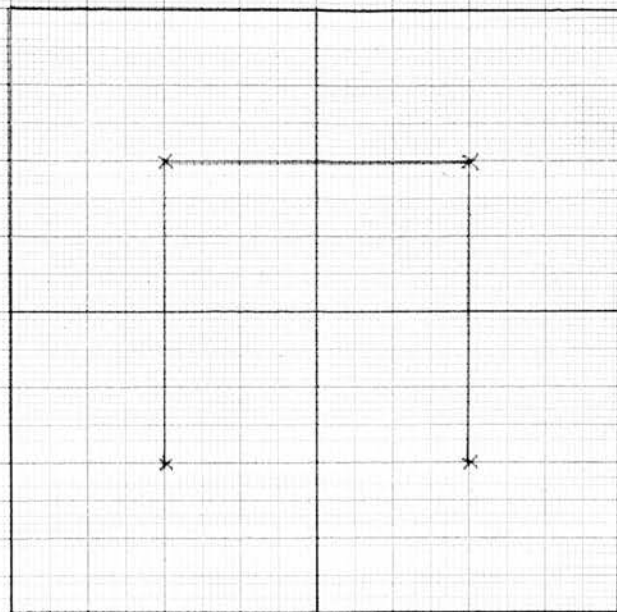


FIG. 2

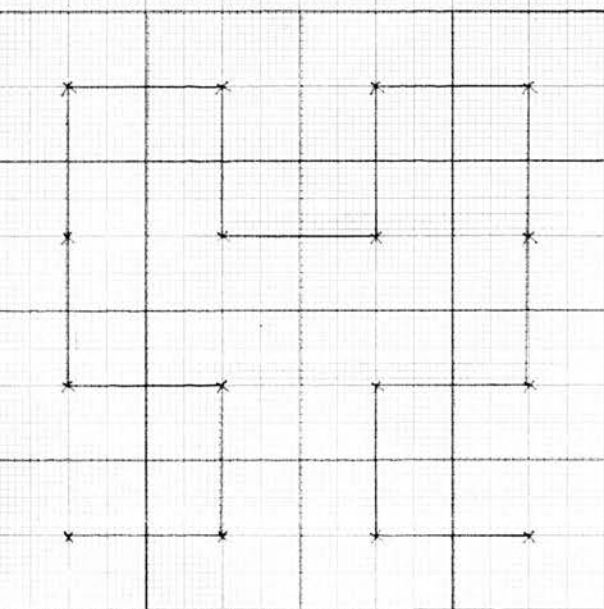


FIG. 3

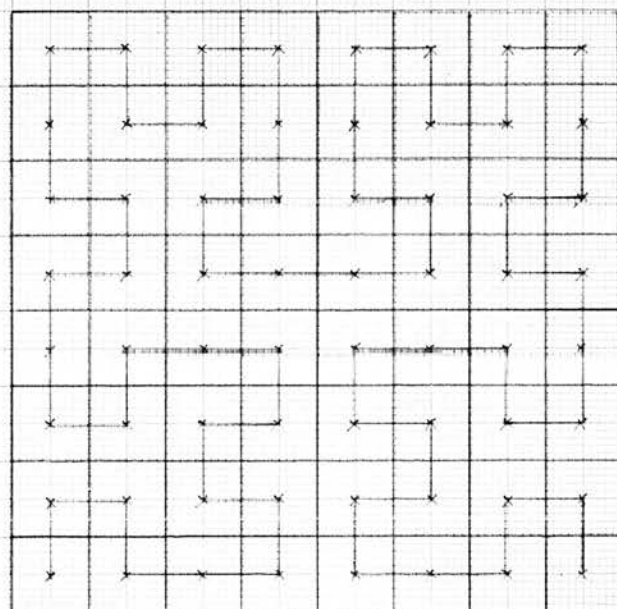


FIG. 4

that Hilbert's curve is obtained as the limit of a sequence of polygonal stretches. There are three steps that definitely determine the curve, viz.,

(i) The unit square is divided into 2^2 parts and the central points of the new squares are joined by straight lines parallel to the sides of the square. Each sub-square is then further sub-divided into 2^2 parts and again the central points are joined one to the next by straight lines parallel to the sides. This process is continued at infinitum each time creating a new curve cancelling the previous one.

(ii) The central points are joined in this way that the curve passes to the next original square only when it has passed through all the four new sub-squares of each of the previous original squares.

(iii) The continuity of the curve is maintained.

Our analytically given curve will now be shown to possess these properties.

1. From the definitions (1.4) and (1.5), b , and c , are both equal to +1. They together represent the central point of the square (fig. 1). Next b_1 can be either +1 or -1; similarly c_1 is either +1 or -1. Thus b_1 and c_1 together represent for different combinations with b , and c , the four

central points of the four sub-squares.

Similarly b_{n+1} and c_{n+1} in different combinations with the previous b 's and c 's represent the central points of one and all of the squares obtained at the n th division.

And n approaches infinity.

2. If after the n th stretch we want to consider the $(n+1)$ th we proceed as follows:-

To one and all of the sets of $a_1, a_2, \dots, a_{2n-2}$ we add a_{2n-1} and a_{2n} which are separately 0 or 1. Thus from one of the original sets we get four new sets in which $a_1, a_2, \dots, a_{2n-2}$ have the same values as in the original set. We have also seen that no change in $a_1, a_2, \dots, a_{2n-2}$ means no change in b_1, b_2, \dots, b_n . Four sets of values of a_{2n-1} and a_{2n} give four corresponding sets of combinations of b_{n+1} and c_{n+1} which means that the four new central points of the new sub-squares are obtained. So, as one passes from one original t point to the next original t point, one has to pass through the four new t points obtained at the $(n+1)$ th division. Hence in passing from one original square to the next original square one has to pass through the four new sub-squares of the original square from which one is passing to the next.

3. From the proof of the continuity of $f_1(t)$ and $f_2(t)$ it can be seen at once that the finite stretches are also continuous.

Thus it has been shown that the analytically given curve represents Hilbert's space-filling curve.

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ON THE POTENTIAL OF BODIES WITH DISCONTINUOUS
DENSITIES.

ON THE POTENTIAL OF BODIES WITH DISCONTINUOUS DENSITIES.*

INTRODUCTION.

The object of the present paper is to consider the question of the existence of the second derivative of the potential of a body at a point inside it when the density of the body has discontinuities of the second kind at that particular point.

The well known Poisson's equation

$$\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2} = -4\pi\rho$$

was obtained under the consideration that the density was constant in the neighbourhood, or, however small,

of the point (x, y, z) . Gauss (1840) showed that the same equation will hold even if ρ be not constant.

If ρ is a function of (x, y, z) it should be finite and continuous together with its three partial derivatives of the first order.

Later on mathematicians wanted to impose still less strict conditions on ρ and Hölder (1882) showed that ρ should satisfy only this condition viz.,

$$|\rho(\xi, \eta, \zeta) - \rho(x, y, z)| < A r^\mu,$$

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λ and μ being positive constants and r the distance between (ξ, η, ζ) and (x, y, z) . Later Morera (1887) established the equation if

$$\lim_{r \rightarrow 0} \int_0^r \rho(\xi, \eta, \zeta) - \rho(x, y, z) \} \frac{dr}{r}$$

is finite. Henrik Petrinì treated the whole question of potentials and their various derivatives in a masterly memoir (1908) and showed that the Poisson's equation will be satisfied under the only condition that ρ is continuous, but the form of the Poisson's equation has to be modified to suit the needs; it is

$$\lim_{h_p \rightarrow 0} \sum_{p=1}^3 \frac{1}{h_p} \left[\frac{\partial V(x+h_p, y, z)}{\partial x} - \frac{\partial V(x, y, z)}{\partial x} \right] = -4\pi\rho$$

where $\frac{h_p}{h_\mu} \neq 0$ and is determinate. There are cases

e.g. $\rho = \frac{\cos \theta}{\log r}$ where $\frac{\partial^2 V}{\partial x^2}$ etc. do not exist separately

at the origin although ρ is continuous there, and still

the Poisson's equation in the generalised form is

satisfied. Petrinì also obtained the condition necessary

for the existence of the second derivative $\frac{\partial^2 V}{\partial x^2}$ in

the form that

$$\lim_{h \rightarrow 0} \int_0^{2\pi} d\psi \int_{-1}^1 (3\mu^2 - 1) d\mu \int_h^a \rho \frac{dr}{r}$$

should exist and be finite.

G. Prasad (1916) was the first to consider the case of the existence of the second derivatives of the potential when the density was not continuous. He has considered the cases when ρ is of the form

$$\rho = \cos f(r) \text{ or } \cos f(x)$$

where

$$f(\xi) \sim \log \frac{1}{\xi} ,$$

and has shown that the second derivative $\frac{\partial^2 V}{\partial x^2}$ exists but only if this last condition is satisfied.

In this paper taking the polar coordinates of a point to be $r, \cos^{-1} \mu, \psi$, I have considered the cases when $\rho = \cos f(r, \mu, \psi)$. Here the function of f may be any function of r, μ and ψ of the form

$$\frac{1}{F(r) G(\mu) H(\psi)}$$

where neither of the functions $G(\mu)$ and $H(\psi)$ becomes infinite within the range of integration. The discontinuity in ρ may be due to r, μ or ψ or all of them.

My thanks are due to Prof. G. Prasad for suggesting the problem to me and taking interest in my work.

§1.

Let O be the point at which we require the second derivatives of the potential of a body with density having discontinuities of the second kind. Let us surround O by a small sphere of radius a and let O be the origin of coordinates. Then V the potential of this sphere at O is given by

$$(1.1) \quad V = \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^a \rho r dr,$$

where $\mu = \cos \theta$.

Also the potential at $(h, 0, 0)$ is

$$(1.2) \quad V_h = \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^a \rho r^2 \frac{dr}{R}$$

where

$$(1.3) \quad R = (r^2 - 2r\mu + h^2)^{\frac{1}{2}}$$

$$(1.4) \quad \frac{\partial V}{\partial x} = \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^a \rho dr$$

and

$$(1.5) \quad \frac{\partial V_h}{\partial x} = \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^a \rho \frac{r\mu - h}{R^3} r^2 dr$$

Let us introduce two new variables t and q given by

$$(1.6) \quad r = ht, \quad q = (t^2 - 2t\mu + 1)^{\frac{1}{2}};$$

then we get

$$(1.7) \quad \frac{1}{h} \left(\frac{\partial V_h}{\partial x} - \frac{\partial V}{\partial x} \right) = \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^1 \rho \left(\frac{t\mu - 1}{q^3} t^2 - \mu \right) dt \\ + \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_1^{a/h} \rho \left(\frac{t\mu - 1}{q^3} t^2 - \mu \right) dt,$$

the range of integration having been split in two parts.

Now the existence of the right hand side of the equation (1.7) depends upon the existence of its two terms as convergent integrals. And as ρ always lies between $+1$ and -1 being equal to $\cos f(r, \mu, \psi)$, although it may have infinite number of oscillations, we may just examine whether

$$(1.8) \quad \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^1 \left| \frac{t\mu - 1}{q^3} t^2 - \mu \right| dt$$

and

$$(1.9) \quad \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_1^{a/h} \left| \frac{t\mu - 1}{q^3} t^2 - \mu \right| dt$$

and

$$(1.10) \quad \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^1 \rho dt$$

exist as definite convergent integrals.

§2.

We consider the integration with respect to t first. Let us introduce abbreviations

$$(2.1) \quad L = \int_0^1 \left(\frac{t\mu-1}{q^3} t^2 - \mu \right) dt ,$$

$$(2.2) \quad L_k = \int_0^{q/k} \left(\frac{t\mu-1}{q^3} t^2 - \mu - \frac{3\mu^2-1}{t} \right) dt ,$$

$$(2.3) \quad K_k = \int_0^{q/k} \frac{3\mu^2-1}{t} dt ;$$

and let

$L(w)$ represent the indefinite integral L where t has been replaced by w . Thus the conditions (1.8) and (1.9) become that the following three integrals should be convergent:

$$\int_0^{2\pi} d\psi \int_{-1}^1 L d\mu , \quad \int_0^{2\pi} d\psi \int_{-1}^1 L_k d\mu , \quad \int_0^{2\pi} d\psi \int_{-1}^1 K_k d\mu .$$

Equation (1.7) is now

$$(2.4) \quad \frac{1}{k} \left(\frac{\partial V_k}{\partial x} - \frac{\partial V}{\partial x} \right) = \int_0^{2\pi} d\psi \int_{-1}^1 (L + L_k + K_k) d\mu .$$

In the evaluation of the above integrals we take help of two known integrals (see Petrini, p 323) viz.,

$$(2.5) \quad \int \frac{t^3}{q^3} dt = q + 3\mu \log(q + t - \mu) + \frac{(4\mu^2-3)\mu t + 1 - 2\mu^2}{(1-\mu^2)q}$$

$$(2.6) \quad \int \frac{t^2}{q^3} dt = \log(q + t - \mu) + \frac{(2\mu^2-1)t - \mu}{(1-\mu^2)q} .$$

We therefore obtain after a little rearrangement

$$(2.7) \quad L_h(w) = \mu(w^2 - 2\mu w + 1)^{\frac{1}{2}} + (3\mu^2 - 1) \log \left(\frac{(w^2 - 2\mu w + 1)^{\frac{1}{2}} + w - \mu}{w} \right) \\ - \mu w + \frac{(1 - 4\mu^2)w + 2\mu}{(w^2 - 2\mu w + 1)^{\frac{1}{2}}} ,$$

$$(2.8) \quad L_h(1) = (3\mu^2 - 1) \log \{ (2 - 2\mu)^{\frac{1}{2}} + 1 - \mu \} - \mu \\ + (2 - 2\mu)^{\frac{1}{2}} \mu + \frac{1 + 2\mu - 4\mu^2}{(2 - 2\mu)^{\frac{1}{2}}} ,$$

and

$$(2.9) \quad \lim_{h \rightarrow 0} L_h\left(\frac{a}{k}\right) = (1 - 4\mu^2) + (3\mu^2 - 1) \log 2 .$$

Further

$$(2.10) \quad L(1) = L_h(1) ,$$

and

$$(2.11) \quad L(0) = 3\mu + (3\mu^2 - 1) \log(1 - \mu) .$$

Some of the above results become infinite when $\mu = 1$ but all of them have convergent integrals with respect to u , e.g.,

$$\int (3\mu^2 - 1) \log(1 - \mu) d\mu \\ = (\mu^3 - \mu) \log(1 - \mu) + \int \frac{\mu^3 - \mu}{1 - \mu} d\mu \\ = -\mu(1 + \mu)(1 - \mu) \log(1 - \mu) - \frac{\mu^2}{2} - \frac{\mu^3}{3} ,$$

and if in this we substitute $\mu = 1$ the result is finite. Similarly we can deal with the expression (2.8). These results show that if ^{we} divide the range of integration into a suitable number of finite parts in which the integrands do not change sign and sum these integrals

which are all finite we have

$$\int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^1 \left| \frac{t^{\mu-1}}{q^3} t^2 - \mu \right| dt$$

and

$$\int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_a^h \left| \frac{t^{\mu-1}}{q^3} t^2 - \mu - \frac{3\mu^2-1}{t} \right| dt$$

as finite quantities, and therefore also

$$\int_0^{2\pi} d\psi \int_{-1}^1 L d\mu \quad \text{and} \quad \int_0^{2\pi} d\psi \int_{-1}^1 L_h d\mu$$

We have now to deal with K_h or rather with

$$(2.12) \quad \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_1^{a/h} (3\mu^2 - 1) \rho \frac{dt}{h}$$

and (1.10). So, we have reduced the problem of the existence of $\frac{\partial^2 v}{\partial x^2}$ to depend upon the finiteness of (2.12) and (1.10).

§3.

We now consider the integrals mentioned above with different possibilities of ρ as a function of r , μ and ψ . Transforming back to the variable r we can write (2.12) and (1.10) as

$$(3.1) \quad \int_0^{2\pi} d\psi \int_{-1}^1 (3\mu^2 - 1) d\mu \int_h^a \rho \frac{dr}{r}$$

and

$$(3.2) \quad \int_0^{2\pi} d\psi \int_{-1}^1 d\mu \int_0^h \rho \frac{dr}{h}$$

Case 1.

Let ρ be a function of r alone.

In this case (3.1) is identically zero because of $\int_{-1}^1 (3\mu^2 - 1) d\mu$ being zero; and (3.2) becomes

$$(3.3) \quad \frac{4\pi}{h} \int_0^h \cos f(r) dr$$

This case has been treated fully by G. Prasad (1916); he has shown that the necessary and sufficient condition for the existence of the integral (3.3) is that

$$(3.4) \quad f(r) \asymp \log \frac{1}{r} \quad \text{when } r \rightarrow 0.$$

Case 2. Let ρ be a function of r and ψ . Again (3.1) is identically zero and (3.2) becomes

$$(3.5) \quad 2 \int_0^{2\pi} d\psi \int_0^h \cos f(r, \psi) \frac{dr}{h}$$

We shall consider this integral later on.

Case 3. Let ρ be independent of r . There are two possibilities: (1) ρ as a function of ψ alone; (2) ρ as a function of μ and ψ . The first possibility is only a particular case of case 2.

As the integral

$$\int_0^{2\pi} d\psi \int_{-1}^1 (3\mu^2 - 1) \cos(\mu, \psi) d\mu$$

is definitely different from zero,

$$\lim_{h \rightarrow 0} \int_0^{2\pi} d\psi \int_{-1}^1 (3\mu^2 - 1) \cos(\mu, \psi) d\mu \int_h^a \frac{dr}{r}$$

is infinite.

In this case therefore $\frac{\partial^2 V}{\partial x^2}$ does

not exist.

Case 4. Let ρ be a function of all the variables i.e. let it be of the form

$$(3.6) \quad \rho = \cos \frac{1}{F(r) G(\mu) H(\psi)}$$

It is easy to see that the convergence of (3.1) and (3.2) depends upon the convergence of

$$\int_0^h \cos \frac{1}{F(r) G(\mu) H(\psi)} \frac{dr}{h}$$

and

$$\int_h^a \cos \frac{1}{F(r) G(\mu) H(\psi)} dr$$

i.e.

$$(3.7) \quad \int_0^h \cos \frac{1}{A F(r)} \frac{dr}{h} \quad \text{and} \quad \int_h^a \cos \frac{1}{A F(r)} dr ,$$

where A is independent of r. And for the convergence of both the integrals in (3.7) it is necessary and sufficient that

$$\frac{1}{F(r)} \sim \log \frac{1}{r} \quad \text{when } r \rightarrow 0,$$

and A should not become infinite which means that neither of the functions $G(\mu)$ and $H(\psi)$ should become infinite within the range of integration.

Case 2 is a particular case of case 4, i.e. when $G(\mu)$ is constant.

We now conclude by obtaining the following results:-

1. When ρ is a function of r of the form

$$\rho = \cos \frac{1}{F(r) G(\mu) H(\psi)}$$

where $G(\mu)$ and $H(\psi)$ are not infinite for any values of μ and ψ within the range of integration it is necessary and sufficient for the existence of the second derivative $\frac{\partial^2 v}{\partial x^2}$ that

$$\frac{1}{F(r)} \sim \log \frac{1}{r}$$

2. When ρ is independent of r and $G(\mu)$ is not a constant then $\frac{\partial^2 v}{\partial x^2}$ does not exist.

3. When ρ is independent of both r and μ then $\frac{\partial^2 v}{\partial x^2}$ exists $H(\psi)$ being any function of ψ .

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ON THE EXPANSION OF $\theta_n(h)$ IN THE LAGRANGE'S
REMAINDER.

ON THE EXPANSION OF $\Theta_n(h)$ IN THE LAGRANGE'S REMAINDER.*

INTRODUCTION

The problem of finding an expansion for $\Theta(h)$ in powers of h in the form

$$\Theta(h) = \sum_{n=0}^{\infty} A_n h^n$$

on the assumption that $f(x)$ is unlimitedly differentiable and $f''(x)$ is different from zero engaged the attention of Whitcomb (4) as early as 1880 and has since then been considered by a number of well-known mathematicians viz., R. Rothe (3), T. Hayashi (1) and others; but it was reserved to B.N. Pal (2) to go a step further than Whitcomb by giving the coefficients of powers of h in the expansion of $\Theta(h)$ of the mean-value theorem up to A_7 .

The present paper is the outcome of my attempt to obtain the general term in the expansion of $\Theta_n(h)$.

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I have calculated coefficients up to A_9 and it has been shown that a general form for the coefficients can be given and it is

$$A_m = \sum K_m \phi_{a_1}^{\alpha_1} \cdot \phi_{a_2}^{\alpha_2} \cdots \phi_{a_r}^{\alpha_r},$$

the summation extending to all possible positive and integral values of α 's and a 's subject to the condition that

$$\sum_{q=1}^r a_q \alpha_q = m.$$

The constant K_m is to be determined. The problem of obtaining the numerical factor K_m presents difficulties similar to those in the case of finding the numerical coefficients in the expansion of $\wp(z)$ or the Jacobian elliptic functions $\text{sn}(z)$, $\text{cn}(z)$, $\text{dn}(z)$ in powers of the argument z .

This problem was taken up by me at the suggestion of Prof. G. Prasad and I take this opportunity of expressing my sincere thanks to him for the interest he took in my work.

The general expansion of $\theta_n(h)$ in the Lagrangian remainder is taken up in § 1, and a general equation is obtained connecting the first n consecutive coefficients. In § 2 the coefficients of powers of h have been obtained up to the 6th term and the general trend of the result is deduced. In § 3, $\theta(h)$ of the mean-value theorem for $n = 1$

is obtained, coefficients up to the 9th power of h being calculated. Any next higher coefficient can be immediately obtained by substituting the values of the previous ones in the equation (3.1).

§1.

Let

$$(1.1) \quad f(x+h) = f(x) + h f'(x) + \frac{h^2}{2!} f''(x) + \dots \\ \dots + \frac{h^n}{n!} f^{(n)}(x + \theta_n h),$$

and assume $f(x+h)$ to be expansible in the series

$$(1.2) \quad f(x+h) = \sum_{m=0}^{\infty} f^{(m)}(x) \frac{h^m}{m!},$$

and also

$$(1.3) \quad f^{(n)}(x + \theta_n h) = \sum_{p=0}^{\infty} f^{(n+p)}(x) \frac{(\theta_n h)^p}{p!}$$

and also assume θ_n to be expansible in the series

$$(1.4) \quad \theta_n = \sum_{r=0}^{\infty} A_r h^r.$$

From (1.1), (1.2) and (1.3) we get the equality

$$(1.5) \quad \sum_{m=0}^{\infty} f^{(m)}(x) \frac{h^m}{m!} = \sum_{p=0}^{n-1} f^{(p)}(x) \frac{h^p}{p!} \\ + \frac{h^n}{n!} \sum_{p=0}^{\infty} f^{(n+p)}(x) \frac{(\theta_n h)^p}{p!},$$

and using (1.4) for θ_n we get

$$(1.6) \quad \sum_{m=0}^{\infty} f^{(m)}(x) \frac{h^m}{m!} = \sum_{p=0}^{n-1} f^{(p)}(x) \frac{h^p}{p!} \\ + \frac{h^n}{n!} \sum_{p=0}^{\infty} f^{(n+p)}(x) \left\{ \sum_{r=0}^{\infty} A_r h^r \right\}^p.$$

Now $\{ \sum_{r=0}^{\infty} A_r h^r \}^p$ is an infinite series raised to power p . If we want the coefficient of h^q from the series after expansion we need not expand the infinite series, the finite series $\{ \sum_{r=0}^q A_r h^r \}^p$ alone is sufficient for our purpose. Thus the coefficient of h^q is

$$(1.7) \quad \sum \frac{p!}{a_0! a_1! \dots a_q!} A_0^{a_0} A_1^{a_1} \dots A_q^{a_q}$$

where a 's have all possible positive integral values subject to the conditions

$$(1.8) \quad \begin{cases} \sum_{r=0}^q a_r = p \\ \sum_{r=1}^q r a_r = q \end{cases}$$

Now equating the coefficients of h^{m+n} on both sides of (1.6) we get

$$(1.9) \quad \frac{f^{(m+n)}}{(m+n)!} = \frac{1}{n!} \sum_{p=0}^n \frac{f^{(n+p)}}{p!} \sum \frac{p!}{a_0! a_1! \dots a_{n-p}!} A_0^{a_0} A_1^{a_1} \dots A_{n-p}^{a_{n-p}}$$

where a 's have all possible positive integral values subject to the conditions

$$(1.10) \quad \sum_{r=0}^{n-p} a_r = p, \quad \sum_{r=1}^{n-p} r a_r = n-p, \quad m \neq 0$$

The following more convenient form of the equation (1.9) is obtained when it is combined with (1.10). Thus

$$(1.11) \quad \frac{n!}{(n+m)!} f^{(n+m)} = f^{(n+1)} A_{m-1} + f^{(n+2)} \left\{ A_{m-2} A_0 + A_{m-3} A_1 + A_{m-4} A_2 + \dots \right\} + f^{(n+3)} \left\{ A_{m-3} \frac{A_0^2}{2!} + A_{m-4} A_0 A_1 + A_{m-5} (A_1 A_0 + \frac{A_1^2}{2!}) + \dots \right\} + \dots + f^{(n+m)} \frac{A_0^n}{n!}$$

This is the equation giving a definite unique relation amongst the different consecutive coefficients including A_0 .

§2

A few coefficients are now obtained to show the general trend of the form of the coefficients
Let us introduce a function

$$(2.1) \quad \phi_p = \frac{f^{(n+p+1)}}{f^{(n+1)}} ,$$

and let

$$(2.2) \quad d_p = \frac{1}{(n+1)^p p!} - \frac{n!}{(n+p)!}$$

with

$$(2.3) \quad d_1 = \frac{1}{n+1} .$$

Then

$$A_0 = \frac{1}{n+1} = d_1 ,$$

$$\begin{aligned} A_1 &= -\phi_1 \left[\frac{1}{(n+1)^2 2!} - \frac{n!}{(n+2)!} \right] \\ &= -\phi_1 d_2 . \end{aligned}$$

$$\begin{aligned} A_2 &= -\phi_1 (A_1 A_0) - \phi_2 \left(\frac{A_0^3}{3!} - \frac{n!}{(n+3)!} \right) \\ &= \phi_1^2 d_1 d_2 - \phi_2 d_3 . \end{aligned}$$

$$\begin{aligned} A_3 &= -\phi_1 \left(A_2 A_0 + \frac{A_1^2}{2} \right) - \phi_2 A_1 \frac{A_0^2}{2} - \phi_3 \left(\frac{A_0^4}{4!} - \frac{n!}{(n+4)!} \right) \\ &= -\phi_1^3 \left(d_1^2 d_2 + \frac{d_2^2}{2} \right) + \phi_1 \phi_2 \left(\frac{d_1^2 d_2}{2} + d_1 d_3 \right) - \phi_3 d_4 . \end{aligned}$$

$$\begin{aligned}
A_4 &= -\phi_1(A_3A_0 + A_2A_1) - \phi_2\left(A_2\frac{A_0^2}{2} + \frac{A_1^2}{2}A_0\right) - \phi_3A_1\frac{A_0^3}{3!} \\
&\quad - \phi_4\left(\frac{A_0^5}{5!} - \frac{n!}{(n+5)!}\right) \\
&= \phi_1^4(d_1^3d_2 + \frac{3}{2}d_1d_2^2) - \phi_1^2\phi_2(d_1^3d_2 + d_1^2d_3 + \frac{d_1d_2^2}{2} + d_2d_3) \\
&\quad + \phi_1\phi_3\left(\frac{d_1^3d_2}{3!} + d_1d_4\right) + \phi_2^2\frac{d_1^2d_3}{2} - \phi_4d_5
\end{aligned}$$

$$\begin{aligned}
A_5 &= -\phi_1(A_4A_0 + A_3A_1 + \frac{A_2^2}{2}) - \phi_2\left(A_3\frac{A_0^2}{2} + A_2A_1A_0 + \frac{A_1^3}{3!}\right) \\
&\quad - \phi_3\left(A_2\frac{A_0^3}{3!} + \frac{A_1^2A_0^2}{2 \cdot 2}\right) - \phi_4\left(A_1\frac{A_0^4}{4!}\right) - \phi_5\left(\frac{A_0^6}{6!} - \frac{n!}{(n+6)!}\right) \\
&= -\phi_1^5(d_1^4d_2 + 3d_1^2d_2^2 + \frac{d_2^3}{2}) + \phi_1^3\phi_2\left(\frac{3}{2}d_1^4d_2 + d_1^3d_3\right. \\
&\quad \left.+ \frac{9}{4}d_1^2d_2^2 + 3d_1d_2d_3 + \frac{d_2^3}{3!}\right) - \phi_1^2\phi_3\left(\frac{1}{3}d_1^4d_2 + \frac{1}{4}d_1^2d_2^2\right. \\
&\quad \left.+ d_1^2d_4 + d_2d_4\right) - \phi_1\phi_2^2\left(\frac{1}{4}d_1^4d_2 + d_1^3d_3 + d_1d_2d_3 + \frac{d_2^2}{3!}\right) \\
&\quad + \phi_1\phi_4\left(\frac{1}{4}d_1^4d_2 + d_1d_5\right) + \phi_2\phi_3\left(\frac{1}{3!}d_1^3d_3 + \frac{d_1^2d_4}{2}\right) - \phi_5d_6
\end{aligned}$$

It is obvious that A_m can be written without difficulty in the form ,

$$(2.4) \quad A_m = \pm \sum K_m \phi_{a_1}^{\alpha_1} \cdot \phi_{a_2}^{\alpha_2} \cdots \phi_{a_r}^{\alpha_r} ,$$

where the summation extends to all possible positive integral values of α 's and a 's subject to the condition

$$(2.5) \quad \sum_{q=1}^r \alpha_q a_q = m ,$$

K_m is a numerical constant to be determined, the sign prefixed being positive or negative as the number of ϕ 's in the term is even or odd. Any particular d may be numerically positive or negative, depending upon n and p .

The difficulty of calculating the K 's becomes obvious when they are calculated for the simplest case viz $n=1$.

§3

Putting $n=1$ in the equation (1.9)

we get

$$(3.1) \quad \frac{f^{(1+m)}}{(1+m)!} = \sum_{p=1}^m f^{(1+p)} \sum \frac{A_0^{\alpha_0} A_1^{\alpha_1} \cdots A_{m-p}^{\alpha_{m-p}}}{a_0! a_1! \cdots a_{m-p}!}$$

α 's obeying condition (1.10). The simpler form (1.11) becomes

$$\begin{aligned}
 (3.2) \quad \frac{f^{(1+m)}}{(1+m)!} &= f^{(2)} A_{m-1} + f^{(3)} (A_{m-2} A_0 + A_{m-3} A_1 + \dots) \\
 &+ f^{(4)} (A_{m-3} \frac{A_0^2}{2!} + A_{m-4} A_1 A_0 + \dots) \\
 &\dots \\
 &+ f^{(m+1)} \frac{A_0^m}{m!} .
 \end{aligned}$$

Putting ϕ_p for $\frac{f^{(p+2)}}{f^{(2)}}$, we get-

$$A_0 = \frac{1}{2} ,$$

$$A_1 = \frac{1}{2^3 \cdot 3} \phi_1 ,$$

$$A_2 = \frac{1}{2!} \left(-\frac{1}{2^3 \cdot 3} \phi_1^2 + \frac{1}{2^3 \cdot 3} \phi_2 \right) ,$$

$$A_3 = \frac{1}{3!} \left(\frac{11}{2^6 \cdot 3} \phi_1^3 + \frac{7}{2^5} \phi_1^2 \phi_2 + \frac{11}{2^6 \cdot 5} \phi_3 \right) ,$$

$$A_4 = \frac{1}{4!} \left(-\frac{3}{2^5} \phi_1^4 + \frac{7}{2^5} \phi_1^2 \phi_2 - \frac{43}{2^5 \cdot 3 \cdot 5} \phi_1 \phi_3 - \frac{1}{2^4} \phi_2^2 + \frac{13}{2^5 \cdot 3 \cdot 5} \phi_4 \right) ,$$

$$\begin{aligned}
 A_5 = \frac{1}{5!} &\left(\frac{5 \cdot 37}{2^7 \cdot 3^2} \phi_1^5 - \frac{5 \cdot 11}{2^2 \cdot 3^3} \phi_1^3 \phi_2 + \frac{3 \cdot 5}{2^6} \phi_1^2 \phi_3 \right. \\
 &\left. + \frac{5}{2^4} \phi_1 \phi_2^2 - \frac{31}{2^7 \cdot 3} \phi_1 \phi_4 - \frac{53}{2^7 \cdot 3} \phi_2 \phi_3 + \frac{19}{2^7 \cdot 7} \phi_5 \right) ,
 \end{aligned}$$

$$\begin{aligned}
 A_6 = \frac{1}{6!} & \left(-\frac{5 \cdot 17}{2^7 \cdot 3} \phi_1^6 + \frac{5^2 \cdot 47}{2^7 \cdot 3^2} \phi_1^4 \phi_2 - \frac{331}{2^6 \cdot 3^2} \phi_1^3 \phi_3 - \frac{5 \cdot 41}{2^6 \cdot 3} \phi_1^2 \phi_2^2 \right. \\
 & + \frac{3 \cdot 5}{2^6} \phi_1^2 \phi_4 + \frac{47}{2^6} \phi_1 \phi_2 \phi_3 - \frac{1}{2 \cdot 7} \phi_1 \phi_5 + \frac{5}{2^5} \phi_2^3 - \frac{3^2}{2^6} \phi_2 \phi_4 \\
 & \left. - \frac{11}{2^7} \phi_3^2 + \frac{3 \cdot 5}{2^7 \cdot 7} \phi_6 \right) ,
 \end{aligned}$$

$$\begin{aligned}
 A_7 = \frac{1}{7!} & \left(-\frac{5 \cdot 7^2 \cdot 11}{2^{10} \cdot 3^2} \phi_1^7 - \frac{5 \cdot 7 \cdot 457}{2^{10} \cdot 3^3} \phi_1^5 \phi_2 + \frac{7 \cdot 11 \cdot 719}{2^{10} \cdot 3^3} \phi_1^4 \phi_3 \right. \\
 & + \frac{5^4 \cdot 7}{2^8 \cdot 3^2} \phi_1^3 \phi_2^2 - \frac{7 \cdot 13 \cdot 61}{2^{10} \cdot 3^2} \phi_1^3 \phi_4 - \frac{7 \cdot 1039}{2^{10} \cdot 3} \phi_1^2 \phi_2 \phi_3 \\
 & + \frac{19 \cdot 37}{2^{10} \cdot 3} \phi_1^2 \phi_5 - \frac{5 \cdot 7 \cdot 19}{2^8 \cdot 3} \phi_1 \phi_2^3 + \frac{7 \cdot 29}{2^8} \phi_1 \phi_2 \phi_4 \\
 & + \frac{7 \cdot 2017}{2^{10} \cdot 3 \cdot 5} \phi_1 \phi_3^2 - \frac{97}{2^9 \cdot 3} \phi_1 \phi_6 + \frac{7 \cdot 41}{2^9} \phi_2^2 \phi_3 - \frac{71}{2^9} \phi_2 \phi_5 \\
 & \left. - \frac{5 \cdot 7 \cdot 17}{2^{10} \cdot 3} \phi_3 \phi_4 + \frac{13 \cdot 19}{2^{10} \cdot 3^2} \phi_7 \right) ,
 \end{aligned}$$

$$\begin{aligned}
 A_8 = \frac{1}{8!} & \left(\frac{5 \cdot 7 \cdot 491}{2^9 \cdot 3^2} \phi_1^8 - \frac{5 \cdot 7 \cdot 541}{2^9 \cdot 3} \phi_1^6 \phi_2 + \frac{7 \cdot 1103}{2^9 \cdot 3^2} \phi_1^5 \phi_3 \right. \\
 & + \frac{5^2 \cdot 7 \cdot 431}{2^8 \cdot 3^3} \phi_1^4 \phi_2^2 + \frac{7 \cdot 1669}{2^9 \cdot 3^2} \phi_1^4 \phi_4 + \frac{7 \cdot 61}{2^7 \cdot 3^2} \phi_1^3 \phi_2 \phi_3 \\
 & - \frac{2141}{2^7 \cdot 3^3} \phi_1^3 \phi_5 - \frac{5 \cdot 7 \cdot 11}{2^6 \cdot 3} \phi_1^2 \phi_2^3 - \frac{7 \cdot 193}{2^6 \cdot 3^2} \phi_1^2 \phi_2 \phi_4 \\
 & \left. - \frac{7 \cdot 17 \cdot 73}{2^9 \cdot 3 \cdot 5} \phi_1^2 \phi_3^2 + \frac{41}{2^6 \cdot 3} \phi_1^2 \phi_6 - \frac{7 \cdot 17}{2^6} \phi_1 \phi_2^2 \phi_3 \right)
 \end{aligned}$$

$$\begin{aligned}
& + \frac{11 \cdot 29}{2^7 \cdot 3} \phi_1 \phi_2 \phi_5 + \frac{3^3 \cdot 7^2}{2^6 \cdot 5} \phi_1 \phi_3 \phi_4 - \frac{7 \cdot 37}{2^9 \cdot 3^2} \phi_1 \phi_7 \\
& - \frac{5 \cdot 7}{2^6 \cdot 3^2} \phi_2^4 + \frac{7 \cdot 11}{2^7} \phi_2^2 \phi_4 + \frac{7 \cdot 29 \cdot 4^3}{2^9 \cdot 3 \cdot 5} \phi_2 \phi_3^2 \\
& - \frac{13}{2^5 \cdot 3} \phi_2 \phi_6 - \frac{3 \cdot 89}{2^8 \cdot 5} \phi_3 \phi_5 - \frac{7 \cdot 13}{2^8 \cdot 3} \phi_4^2 + \frac{251}{2^9 \cdot 3^2 \cdot 5} \phi_8 \Big) ,
\end{aligned}$$

$$\begin{aligned}
A_9 = & \frac{1}{9!} \Big(- \frac{5 \cdot 7 \cdot 23 \cdot 199}{2'' \cdot 3} \phi_1^9 + \frac{5 \cdot 7 \cdot 5171}{2^9 \cdot 3} \phi_1^7 \phi_2 - \frac{7 \cdot 29^3}{2^4 \cdot 3} \phi_1^6 \phi_3 \\
& - \frac{5 \cdot 7 \cdot 11 \cdot 13 \cdot 79}{2^8 \cdot 3^2} \phi_1^5 \phi_2^2 + \frac{7 \cdot 103 \cdot 131}{2'' \cdot 3^2} \phi_1^5 \phi_4 \\
& + \frac{5 \cdot 7^2 \cdot 11 \cdot 59}{2''} \phi_1^4 \phi_2 \phi_3 + \frac{13 \cdot 311}{2'' \cdot 3} \phi_1^4 \phi_5 + \frac{5^2 \cdot 7 \cdot 389}{2^8 \cdot 3} \phi_1^3 \phi_2^3 \\
& - \frac{7 \cdot 11 \cdot 19}{2^8} \phi_1^3 \phi_2 \phi_4 - \frac{7 \cdot 13 \cdot 673}{2'' \cdot 5} \phi_1^3 \phi_3^2 - \frac{461}{2^6 \cdot 3} \phi_1^3 \phi_6 \\
& - \frac{7 \cdot 2749}{2^9} \phi_1^2 \phi_2^2 \phi_3 - \frac{31 \cdot 37}{2^9} \phi_1^2 \phi_2 \phi_5 - \frac{7 \cdot 11 \cdot 19}{2^{10}} \phi_1^2 \phi_3 \phi_4 \\
& + \frac{7 \cdot 191}{2'' \cdot 3} \phi_1^2 \phi_7 - \frac{5 \cdot 7 \cdot 19}{2^6} \phi_1 \phi_4^2 - \frac{7}{2^8} \phi_1 \phi_2^2 \phi_4 - \frac{3 \cdot 7 \cdot 67}{2^{10} \cdot 5} \phi_1 \phi_2 \phi_8 \\
& + \frac{3 \cdot 37}{2^7} \phi_1 \phi_2 \phi_6 + \frac{3^2 \cdot 317}{2^9 \cdot 5} \phi_1 \phi_3 \phi_5 + \frac{3 \cdot 7 \cdot 71}{2^9 \cdot 5} \phi_1 \phi_4^2 - \frac{11 \cdot 47}{2'' \cdot 5} \phi_1 \phi_8 \\
& + \frac{7^2 \cdot 11}{2^8} \phi_2^3 \phi_3 + \frac{3 \cdot 53}{2^8} \phi_2^2 \phi_5 + \frac{3 \cdot 7 \cdot 71}{2^8 \cdot 5} \phi_2 \phi_3 \phi_4 - \frac{271}{2''} \phi_2 \phi_7 \\
& + \frac{3 \cdot 7^2 \cdot 11}{2'' \cdot 5} \phi_3^3 - \frac{3 \cdot 13 \cdot 29}{2^{10} \cdot 5} \phi_3 \phi_6 - \frac{3 \cdot 467}{2^{10} \cdot 5} \phi_4 \phi_5 \\
& + \frac{1013}{2'' \cdot 5 \cdot 11} \phi_9 \Big) .
\end{aligned}$$

Similarly A_0 and others can be obtained. It is evident that every next higher coefficient may be calculated by substituting the values of the lower ones in the equation (3.2) but the tediousness of the calculation is obvious.

As regards the general law of the coefficient A_m the following remarks can be made on the basis of equations (1.9) and (1.11) :-

(i) The equations give a relation between all the first $(m - p)$ A's.

(ii) The sum of the suffixes of A's is equal to $m - p$; in other words the sum of the suffixes of the A's together with the suffix of the accompanying f is equal to the suffix of the f on the left hand side of the equation.

(iii) Any A raised to a power is accompanied by a factorial of the power in the denominator.

(iv) The number of A's in any term is p . It is less by n than the suffix of the accompanying f .

(v) The number of terms for particular values of m and p is $P(m - p | p|)$.

By putting $m=1$, we get an equation giving A_0 . Then $m = 2$ gives us an equation in which if we substitute the value of A_0 we get A_1 . In this way by giving in succession to m the values $1, 2, 3, \dots$ we get a set of equations involving A_0, A_1, A_2, \dots , and by substituting the previously obtained values of A's we get the next higher A.

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